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Theme:

Magnetic Susceptibility in the Ising Model

Presented by

Ala Ouguergouz

Presented the $29^{t\Box}$ of September 2019 under the examining committee:

Dr. Mouzali Aziz **MCB** Blida University 1 President Prof. Salah Boukraa Professor Blida University 1 Supervisor Dr. Bahia Si Lakhal **MCA** ENP, El Harrach Examiner Dr. Yahiaoui Sid-Ahmed **MCB** Blida University 1 Examiner

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To the Memory of Professor M. Bentaiba, a great physicist and Humanist

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Abstract

Ferromagnetism emerges when a collection of particle spins align such that their associated magnetic moments all point in the same direction, yielding a macroscopic sized net magnetic moment.

The simplest theoretical description of ferromagnetism was given by the Ising model. This model was invented by Wilhelm Lenz in 1920 and it is named after his student Ernst Ising who introduced it in his PhD thesis in 1925.

Ising has introduced his model by supposing nearest-neighbor interactions between spins on a lattice and an interaction with an external magnetic field H.

Using statistical physics methods, the model has been solved exactly in one dimension (for any H) and in two dimensions (for H=0) and the corresponding free energy and spontaneous magnetization have been obtained in terms of the temperature. In two dimensions, it can be seen that this model can describe and explain phase transition phenomena.

Another quantity of physical interest for this model and which has been widely investigated is the magnetic susceptibility. It has still no clear analytical status, however, we know that it can be expressed as an infinite sum of spin correlation functions.

The aim of our work in this thesis is to present an algorithm, using quadratic recursion relations, which allows the calculations of the analytical expressions of these correlation functions C(M, N) in terms of the temperature for all values of M and N(which represent the position of the spn in a lattice) in the isotopic case (J = J') when the magnetic field is zero (H = 0).

Key Words

Correlation function, Ising model, ferromagnetism, Toeplitz determinants.

Résumé

Le ferromagnétisme apparaît lorsqu'un ensemble de spins de particules s'aligne de telle sorte que leurs moments magnétiques associés pointent tous dans la même direction, ce qui donne un moment magnétique net de taille macroscopique.

La description théorique la plus simple du ferromagnétisme a été donnée par le modèle d'Ising. Ce modèle a été inventé par Wilhelm Lenz en 1920 et porte le nom de son étudiant Ernst Ising qui l'a introduit dans sa thèse de doctorat en 1925.

Ising a introduit son modèle en supposant des interactions entre spins voisins les plus proches sur un réseau et une interaction avec un champ magnétique externe H.

En utilisant des méthodes de physique statistique, le modèle a été résolu exactement en une dimension (pour tout H) et en deux dimensions (pour H=0) et l'énergie libre et l'aimantation spontanée correspondantes ont été obtenues en termes de température. En deux dimensions, on peut voir que ce modèle peut décrire et expliquer les phénomènes de transition de phase. Une autre quantité d'intérêt physique pour ce modèle, qui a fait l'objet de nombreuses recherches,

est la susceptibilité magnétique. Elle n'a toujours pas de statut analytique clair, mais nous savons qu'elle peut s'exprimer sous la forme d'une somme infinie de fonctions de corrélation de spin.

Le but de notre travail dans cette thèse est de présenter un algorithme utilisant des relations de récurrence quadratiques, qui permet de calculer les expressions analytiques de ces fonctions de corrélation C(M,N) en termes de température pour toutes les valeurs de M et de N dans le cas isotopique (J=J') lorsque le champ magnétique est nul (H=0).

Mots Clés

Fonction de corrélation, modèle d'Ising, ferromagnétisme, déterminants de Toeplitz.

Dedication

I dedicate this work to my Mother, my Role model which I believe without her I could never be where I am today, To the best man in my life, my dear Father who gave courage, embission and love the Hero of my life and always will be.

To my sweet sister who kept motivating me and pushing me to be the best version of myself, to my little brother and my best friends Yasmine and Khawla. To my grandfather whom always cared about my studies and my life. To my sweet grandmother MIMI whom wish to see her smile soon. To my family and my teachers whom i own my success and the knowledge I have. At the end i hope this work will be a fruitfull addition the coming works in the subject.

Acknowledgments

First and foremost, I want to thank Allah for his huge blessing for me writing this today. And Because that may be my only space to thank in individuals in writing. I'd like to thank my Advisor, Dr. S. Boukraa for giving me his time and the chance to try and learn. I am also thankful for the excellent example he has provided as a successful physicist and professor.

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Introduction

Some materials, such as iron, cobalt or nickel, exhibit a spontaneous magnetization at ordinary temperature. These materials, called ferromagnetic, are characterized by the Curie temperature above which they lose their spontaneous magnetization: a (phase) transition takes place between a ferromagnetic phase and a paramagnetic phase.

Ferromagnetism emerges when a collection of particle spins align such that their associated magnetic moments all point in the same direction, yielding a macroscopic sized net magnetic moment.

To describe this phenomenon, a simple model was proposed by Ising in 1925. He was then a doctoral student of the famous German physicist Wilhelm Lenz, who suggested to him this problem in 1920.

Ising has introduced the model by supposing nearest-neighbor interactions between spins on a (d-dimensional) lattice and an interaction with an external magnetic field H.

Using statistical physics methods, the model has been solved exactly in one dimension (for any H) by Ising and in two dimensions (for H = 0) by Lars Onsager in 1944.

Lars Onsager obtained an analytical solution for the free energy and for the spontaneous magnetization for the Ising model on a (two-dimensional) square lattice in terms of the temperature.

In his doctoral thesis, Ising showed that the system does not exhibit a phase transition in one dimension. However, in two dimensions, it can be seen that this model can describe and explain phase transitions phenomena.

The Onsager solution represents a true milestone in the development of the modern theories of critical phenomena. It was the first time that it was shown that a microscopic model leads to a non-analytic behavior within the framework of equilibrium statistical mechanics.

The magnetic susceptibility of the two-dimensional Ising model has also attracted the attention of many mathematicians and physicists who have worked for more than 60 years in areas of equilibrium statistical mechanics, critical phenomena and phase transitions.

To date, while there is still no solution in a closed form for the expression of the magnetic susceptibility. It is known however that it can be expressed as an infinite sum of spin correlation functions.

We will present in this work some of the properties of the Ising model, among them the magnetic susceptibility and their associated correlations functions.

In the first chapter, we will briefly give a general idea about the position of the model in thermodynamic physics by explaining some approximation methods as well as some concepts that the model is concerned about in particular the important physical concept of phase transition.

LIST OF FIGURES 11

In the second chapter where we will introduce the whole concept of magnetization and its appearance in nature. We will discuss the different types of magnetic materials as well as their proprieties and most importantly the ferromagnetism phase.

In the third chapter, we will introduce the Ising model almost generally recalling its historical background, then we will give its general definition and explain its simple concept. We will then introduce the solution that Ising obtained in one dimension using the transfer matrix method. We will then discusse the exact solution of Onsager that he obtained for a two-dimensional model.

This exact solution will be used as a starting point for our calculations in the next chapter where another quantity of physical interest for the model, which is the magnetic susceptibility, and which has been widely investigated in the last decades by many authors. This quantity has still no clear analytical status, however, we know that it can be expressed as an infinite sum of spin correlation functions.

In the fourth chapter, we will present a useful algorithm, using quadratic recursion relations, which allows the calculations of the analytical expressions of these correlation functions C(M,N) in terms of the temperature for all values of M and N in the isotopic case (J=J') when the magnetic field is zero (H=0).

The method on how to calculate the different correlation functions C(M,N) according to their M and N values is the following. For the diagonal correlation functions C(M,M), a Teoplitz determinant relation is used. The elements a(N) of these determinants are expressed in terms of hypergeometrical functions. Finally, a quadratic recursion relation is used to obtain the remaining non diagonal expressions C(M,N), with M different of N.

We will finally give our concllusions and sone perspectives for future works.

Chapter 1

Phase transitions phenomena

In this chapter we will have a general review on the basics of statistical mechanical concepts necessary to understand the development of the solutions of the Ising model. We start first of all by introducing the basic approximations that made the work of physicists easier and gave more potential to the future of physics in general.

1.1 Background statistical mechanics

Statistical mechanics is one of the oldest and venerable branches of physics which has received the attention of many physicists from the time of Gibbs. Since then it has developed in several directions so that at present it is possible to distinguish at least three different theoretical approaches to the subject [2], Some of the better-known approximation schemes are:

- (i) The foundational approach is concerned with the establishment of the basic and general proprieties and the improvement of the existence of theorems for statistical mechanical systems by accurate mathematical means.
- (ii) The phenomenological approach, and it is concerned with correlating and quantitatively explaining the results of experiments by any available method.
- (iii) The model-building approach, which attempts to gain insight into practical situations by studying simple models (Heisenberg model, Ising model, ...) in which at least some physically interesting quantities may be exactly computed [2].

Each of these approaches has made an enormous contribution for the understanding of the statistical mechanics today. However, many models are still considered incomplete solutions. Therefore, the number of exactly solvable problems in a field depends on the complexity of the subject. For instance, there are unnumbered solved problems in classical mechanics while at the other hand very few in relativistic quantum field theory have ever been exactly solved. The scarcity of solvable models in both statistical mechanics and relativistic quantum field theory is due basically to the fact that, in systems with huge number of components, each one may directly or indirectly impact with enormous number of other particles even if the fundamental interaction in two-body are of short range and it is the purpose to study systems with a large number of particles [5,2].

1.2 Phase Transition and Critical Points

Statistical mechanics is concerned with the average proprieties of mechanical systems. These systems contain huge number of individual components and usually it is hard for the observer to study and control this huge number of individuals unless specifying or measuring a few average proprieties.

Interestingly the relationship between pressure and temperature. To take for example water, If we increase the temperature between 99° C to 101°C, the molecules will start to disassemble and the water turns to steam and that what is known phase transition[8].

On the other hand, phase transition is not the only phenomenon that can occur. Consider a bar of iron immerged completely in a strong magnetic field H which is parallel to its axis. That bar will be completely magnetized. Mathematically, we can express that (M is the magnetization) with +1. We decrease H to zero, M won't disappear but rather than that it will (at zero field) experiences another kind of magnetization that is known as **spontaneous magnetization** M_0 .

More specifically, this magnetization occurs in the state in which a magnetic body has its atomic magnetic moments aligned without being affected by an external magnetic field [22]. We expect molecular forces to be invariant with respect to time reversal. This implies that reversing the field will reverse the magnetization, so M must be an odd function of H. It follows that M(H) must have a graph of the type shown in Fig. 2.1(a), with a discontinuity at H=0. This discontinuity in the magnetization is very like the discontinuity in density at a liquid - gas phase transition.

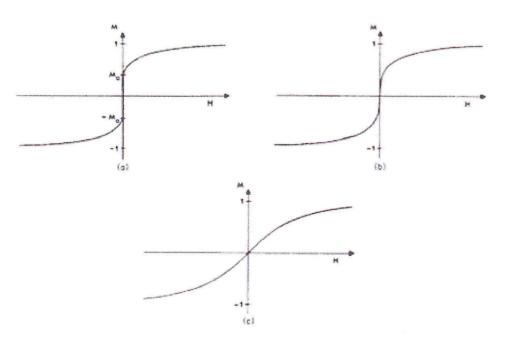


Figure 1.1: Graphs of M(H) shows (a) T<Tc (b) T=Tc (c)T>Tc [9]

The material can be regarded as undergoing a phase Transition at H=0 because it change suddenly from positive to negative magnetization. Moreover, if we increase the temperature T more than the regular temperature, the magnetization M(H) will have a similar graph, but M_0 will be decreased [9]. Eventually, M_0 vanishes if the T increased to a critical value T_c (the Curie point) while M(H) becomes a continuous function with infinite susceptibility at H=0 as shown in Fig.1.1(b).

While in Fig.1.1(c) if T is further increased M(H) remains a continuous function, and becomes analytic at H = 0.

These observations can be summarized by Fig.1.2 and it is a cut along the T axis from 0 to T_c

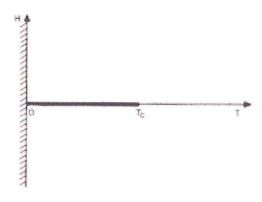


Figure 1.2: The (T,H) half-plane, showing the cut across which M is discontinuous. Elsewhere M is an analytic function of T and H [9].

The cut is a line of phase transitions. Its endpoint $(T_c,0)$ is known as a critical point. Clearly the function M(H,T) must be singular at this point, and one of the most fascinating aspects of statistical mechanics is the study of this singular behaviour near the critical point [9].

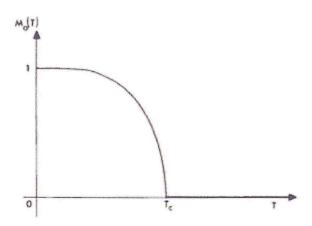


Figure 1.3: The spontaneous magnetization M_0 as a function of temperature [9].

The spontaneous magnetization is a function of T and can be defined as

$$M_0 = \lim_{H \to 0^+} M(H, T)$$

where the limits is taken through the positive values of H. The graph shown in Fig.1.3 is representing the magnetization comparing to the critical temperature T_c , where the spontaneous magnetization M_0 is positive in the case of $T < T_c$ and identically zero for $T > T_c$ [9,3].

1.3 Critical Exponents

The Magnetic Susceptibility is defined by

$$\chi(H,T) = \frac{\partial M(H,T)}{\partial H} \tag{1.1}$$

By taking into consideration the critical behavior, it is convenient to replace T by

$$t = \left(T - T_c\right) / T_c \tag{1.2}$$

And obviously the thermodynamic functions will have singularities at H=0 and t=0 of the form

$$M_{0} \sim (-t)^{\beta} \quad as \quad t \longrightarrow 0^{-}$$

$$M(H, T_{c}) \sim H^{\frac{1}{\delta}} \quad as \quad H \to 0$$

$$\chi(0, T) \sim t^{-\gamma} \quad as \quad t \to 0^{+}$$

$$\chi(0, T) \sim (t)^{-\gamma'} \quad as \quad t \to 0^{-}$$

$$(1.3)$$

The notation $X \sim Y$ is the same as X/Y and it tends to non-zero limits [8] and the powers exponents $\beta, \delta, \gamma, \gamma'$ are numbers, independent of H and T and They are known as the critical exponents.

The first rigorous relation linking critical exponents was derived by Rushbrooke (1963) who, on thermodynamic grounds, showed that for any physical system undergoing a phase transition one has $(\delta+2\beta+\gamma') \geq 2$. The proof of this inequality is straightforward if one adopts a magnetic system as an example [6].

Partition Function

The partition function Z is a fundamental quantity that encompasses the statistical properties of a thermodynamic equilibrium system and it is important for the calculation of other thermodynamic functions such as M(H,T).

Consider a system with states s and Hamiltonian H(s). From the partition function

$$Z = \sum_{s} \exp[-E(s)/kT]$$

k is the Boltzmann's constant and the summation is over all allowed states s of the system. The free energy F is given by [9]:

$$F = kT \ln Z$$

And also the probability of the system being in the state s is

$$P_s = Z^{-1} \exp[-E(s)/kT]$$

The internal energy is:

$$U = \langle E \rangle = Z^{-1} \sum_{s} \exp[-E(s)/kT]$$

that was in general the equations that basically need and see alot in the coming chapter(that was the smily face of these equation and we shall see the evil face later)

By using the partition function and the equation of the free energy we get

$$U = kT^2 \frac{\partial}{\partial T} \ln Z = -T \frac{\partial}{\partial T} (F/T)$$

The basic issue in equilibrium statistics is to evaluate the sum over all states in the partition function. For continuum systems this sum becomes integral. Therefore, the thermodynamic proprieties can be obtained by differentiation. However, the evaluation of Z will be hopelessly difficult in a realistic interacting system in a macroscopic size.

Approximation Methods

In order to simplify our calculations to evaluate the sum-over-states there are some approximations that helps to make it more possible. Some of the better known approximation schemes are:

- (i) Cell or cluster approximations. In these the behaviour of the whole system is extrapolated from that of a very few components inside some 'cell', approximations being made for the interaction of the cell with the rest of the system. Examples are the mean field (Brag and Williams, 1934; Bethe, 1935), they have the advantage of being fairly simple to solve.
- (ii) Approximate integral equations for the correlation functions, notably the Kirkwood 1935 hyper-netted chain (van Leeuwen et al., 1959) and Percus-Yevick. These give fairly good numerical values for thermodynamic proprieties.
- (iii) Computer calculations on systems large on a microscopic scale (e.g. containing a few hundred atoms), but still not of macroscopic size. These calculations evaluate Z by statistically sampling the terms on the RHS of (the partition function above), so are subject to statistical errors, usually of a few per cent. For this reason they are really 'approximations' rather than 'exact calculations'.
- (iv) Series expansions in powers of some appropriate variable, such as the inverse temperature or the density. For very realistic models these can only be obtained to a few terms, but for the three dimensional Ising model expansions have been obtained to as many as 40 terms (Sykes et al., 1965, 1973a)[9].

Chapter 2

Generalities on materials magnetic properties

2.1 Magnetic Proprieties

The magnetic properties of a material are the result of the magnetic propriety of the atoms or ions of these materials. More specifically, the magnetism and magnetization of a material depend on the movement of electrons in an atom. It can thus electron of an atom behaves like a magnet, giving the whole material its magnetic propriety.

2.1.1 Magnetization

The magnetization M is a macroscopic quantity which describes the alignment of particles magnetic moment \overrightarrow{u} in a certain direction. Briefly it is the average of the magnetic moment per site. And it is odd monotonic increasing function of H, lying in the interval $-1 \le M(H,T) \le 1$, see the Fig1.1(a) (first chapter)[8].

Under the magnetic field, magnetic moments in a material tend to align and thus increase the magnitude of the field strength, and that increase is given by the parameter M which is called the magnetization and it is given by:

$$M = \chi_m H \tag{2.1}$$

 χ_m is called Magnetic susceptibility

2.1.2 Spontaneous Magnetization

In general spontaneous magnetization is the appearance of an ordered spin state (magnetization) at zero applied magnetic fields in ferromagnetic or ferromagnetic materials below the critical point called the Curie temperature T_c .

$$M(T) = M(0) \left(1 - \left(\frac{T}{T_c} \right)^{\frac{3}{2}} \right)$$
 (2.2)

M(0) is the spontaneous magnetization at absolute zero.

Near the Curie temperature

$$M \propto (T_c - T)^{\beta} \tag{2.3}$$

 β is the critical exponent that depends on the composition (see chapter 1). Furthermore, the empirical interpolation of the two regimes is given by

$$\frac{M(T)}{M(0)} = \left(1 - \left(\frac{T}{T_c}\right)^{\alpha}\right)^{\beta}$$

and it is convinient to check the two limits of this interpolation that follow laws similar to the Bloch law for $T \to 0$, and the critical behavior, for $T \to T_C$, respectively [31,32].

The SM of IM on a rectangular lattice was first obtained by Onsager in 1948 but he never published his derivation. In 1952 Yang was the first one to publish a derivation for the square lattice[9].

2.1.3 Magnetic susceptibility

By definition the magnetic susceptibility χ_m is the magnetic moment per unit volume and it is a measure for how much a material will become magnetized in an applied magnetic field. Mathematically, it is the ratio of the Magnetization M to the applied magnetizing field intensity H, and it is defined by

$$\chi = \frac{M}{H} \quad (IS) \quad \chi = \frac{\mu_0 M}{H} \tag{2.4}$$

 μ_0 is the vacuum permeability.

This let us simply classify most of materials responding to an applied magnetic field by two ways alignment with the magnetic field into two categories alignment with the magnetic field, $\chi > 0$, called paramagnetism, or an alignment against the field, $\chi < 0$, called diamagnetism [31,32]. The substances of negative magnetic susceptibility are called diamagnetic. The substances of positive magnetic susceptibility are called diamagnetic.

2.1.4 Classes of Magnetic Materials

Above the absolute zero temperature, materials without exception exhibit magnetic susceptibility [5]. The primary distinction is that in some materials, it doesn't exist any collective interaction of atomic magnetic moments, while in other materials exist a very strong interaction between atomic moments[3]. The interaction of a substance with a magnetic field is determined by their magnetic susceptibility which is a dimensionless quantity which expresses the efficiency with which a substance may be magnetized universally. The principal types of interactions can be classified into five major divisions: diamagnetism, paramagnetism, ferromagnetism, ferrimagnetism and antiferromagnetism.

2.1.5 Diamagnetism

Diamagnetism is a fundamental property of all matter, although it is usually very weak [36]. It is due to the non-cooperative behavior of orbiting electrons when exposed to an applied magnetic field. It is important to mention that the diamagnetism is associated with the tendency of electric charges to form a screen between the interior of a body and the applied field [3]. According to Lenz law the variation of a flux through an electrical circuit, an induced current is created in order to oppose this flow variation. The magnetic field produced by the induced current is opposite to the applied field, and the magnetic moment associated with this current is a moment of diamagnetism.

It is axiomatic that two electrons sharing the same orbital, their spin quantum numbers have to be different. Mathematically, one of the electrons has to be "spin-up" $m_s = 1/2$, while the other is "spin-down", with $m_s = -1/2$, and it has an important when it's comes to determining the total spin in an electron orbital. However, when exposed to a field, a negative magnetization is produced and thus the susceptibility is negative. If we plot M vs. H, we see

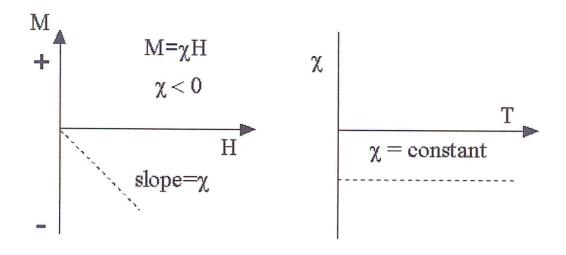


Figure 2.1: Diamagnetism .it shows the behavior of both M and χ in zero magnetic field H [36]

one of the characteristic behavior of diamagnetic materials is that the susceptibility is independent of the temperature as seen in the Fig 2.1.

2.1.6 Paramagnetism

Electronic Paramagnetism (positive contribution to χ) meets [36]:

- i) Atoms, molecules and crystalline defects possessing an odd number of electrons.
- ii) Atoms and free ions of which one internal shell is incomplete.
- iii) Metals

These categories of materials are characteristically famous for their net magnetic moment which exists due to the unpaired electrons in partially filled orbital. One of the most famous atoms with unpaired electrons is iron. However, individual magnetic moments do not interact magnetically. Furthermore, the magnetization goes to zero when there is no an applied magnetic field. Moreover, in the presence of a field it appears a partial alignment of atomic magnetic moments in the same direction of the field, ending up with net positive magnetization and positive susceptibility.

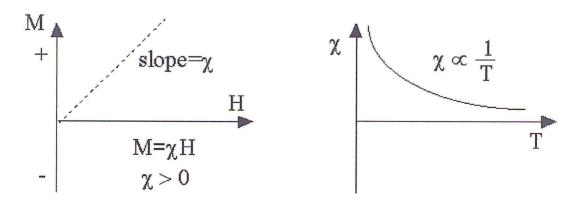


Figure 2.2: Paramagnetism [36]

Additionally, at normal temperatures and in moderate fields, the magnetic susceptibility is independent of the magnetic field either the temperature is very low or the field is high.

2.1.7 Ferromagnetism

A ferromagnetic body has a spontaneous magnetic moment, i.e. magnetic moment (the atomic moments in these materials exhibit very strong interactions¹) even in the absence of an external magnetic field. The presence of a spontaneous moment in a system, suggests that electronic spins and magnetic moments 'of the latter' are arranged in a regular way[10]. the order is not necessarily simple: all the arrangements for ferromagnetism, ferrimagnetisms, except the simple antiferromagnetic have a spontaneous magnetic moment, usually called saturation moment. Ferromagnetic materials exhibit parallel alignment of moments resulting in large net magnetization even in the absence of a magnetic field. And there are obvious characteristics to distinguish ferromagnetic materials from other magnetic materials: Their spontaneous magnetization and the existence of magnetic ordering temperature [36].

parallel alignment

Figure 2.3: Ferromagnetism [36]

2.1.8 Ferrimagnetism

Ferrimagnetisms is a magnetic propriety, where magnetic moments are anti parallel but of different amplitude. This results in a spontaneous magnetization of the material [8], and it is only observed in compounds which have more complex crystal structures than pure elements. Ferrimagnetisms is similar to ferromagnetism, and it exhibits all the hallmarks of ferromagnetic behavior-spontaneous magnetization, Curie temperatures...[5]. However, still have huge difference in their ordering.

2.2 Conclusion

Magnetic Phases transitions A substance may undergo a phase transition from one class to the other, for instance from diamagnetic to paramagnetic at a given temperature, known as Curie temperature. The latter denote a parameter of fundamental importance in magnetic phase transitions.

¹These interactions are produced by electronic exchange forces and result in a parallel or antiparallel alignment of atomic moments

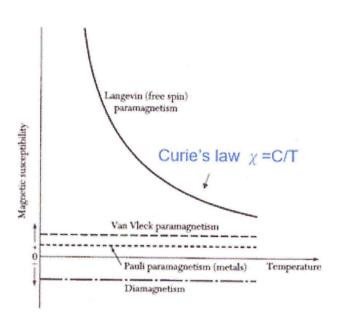


Figure 2.4: Transition Calculation for Ferro-Paramagnetic Lattice [11]

Chapter 3

Ising Model

3.1 Historical survey

Of all systems in statistical mechanics, on which exact calculations have been preformed, the two-dimensional Ising Model is not only the most thoroughly investigated, it is also the richest and most profound.

The Ising Model statistical system has been introduced in 1925 by Ising which bears his name, he studied some of its properties in one-dimension, and it's not until 1941 the quantitative statement about the phase-transition in the two-dimensional was made by Kramer and Wannier and also Montroll who calculated the Curie (Critical) temperature. 1944 the Ising Model was remarkably token to the next level when Onsager was able to compute the thermodynamic proprieties of the two-dimensional lattice in the absence of the external magnetic field.

Then the great simplification of the Onsager's approach was made by Kaufman in 1949 and the same year Onsager's paper about the Spontaneous Magnetization without derivation was published, and then in 1952 Yang published a paper on the first derivation. For the next decade no new result of fundamental significance was derived, but a great deal was accomplished in simplifying the mathematics of these pioneering papers.

The work of Kac, Kasteleyn, Montroll, Potts, Szego and Ward, among others, has been specially significant. The methods of Onsager, Kaufmann and Yang, although very beautiful and powerful, are also extremely complicated. Thus, the two-dimensional Ising Model has acquired a notorious reputation for difficulty whereas, in fact, the simplified methods developed by 1963 have reduced the analysis to the point where it may be readily understood. Since then we have actively used these methods as the basis for computing many more quantities of physical interest [3].

3.2 Definitions

To begin with we need a lattice which for us will be a finite set of regularly spaced points in a space of dimension d = 1, 2 or 3. In one dimension we simply have a string of points on a line, which can enumerate from 1 to N ("N" denote the number of lattice sites, regardless of dimension), in two dimension is usually called the square lattice, in three the cubic lattice (there are lots of other interesting lattices. For example, in two dimensions one can consider the triangular lattice or the hexagonal lattice). At the moment we consider a lattice of magnetic moments. On each lattice sites the local magnetic moment is represented by a "spin". We assume that the spin has just two possible states, either pointing up which is represented by +1 or pointing down which is -1. We use letters like I to denote a site in that lattice. For each site I we have a variable σ_i which only takes on the values +1 and -1 (as mentioned previously). Ultimately we want to work with a full lattice. In the process of doing this we

have to approach the infinite lattice to a finite lattice by and then try to take an "infinite volume limits" in which the finite lattice approaches the full infinite lattice in some sense.

The energy for the IM includes two contributions: the interaction between neighboring spins and the effect of an applied magnetic field on each individual spin. The interaction between neighboring spins tends to induce parallel alignment of the neighbors, so it should be favorable (negative) when the neighbors are both +1 or both -1 and unfavorable (positive) when the neighbors are +1 next to -1. Hence, for each pairs of neighbors i and j, the interaction between two nearest neighbour spins σ_i and σ_j contribute in term $-J\sigma_i\sigma_j$ to the Hamiltonian if they are horizontal neighbours, where J is a positive coefficient giving the interaction strength and $-J'\sigma_i\sigma_j$ if they are vertical neighbours. Where J and J' are some fixed energy.

If the magnetic field H is pointing up, it favors each spin pointing up; if the field energy can be written as $-H\sigma_i$. Putting these pieces together, the local energy for the system becomes [12]

$$E = -J \sum_{(i < j)_{hor}} \sigma_i \sigma_j - J' \sum_{(i < k)_{vert}} \sigma_i \sigma_k - H \sum_i \sigma_i$$
(3.1)

Where the notation $(i,j)_{hor}$ resp. $(i,k)_{vert}$ are the only next-neighbour horizontal and vertical bonds can be included in the summation. Moreover, the sum is over all pairs of sites in our finite volume which are nearest neighbors in the sense that the Euclidean distance between them is 1. The probability measures is given by

$$\mu_{L\to\infty}(\sigma) = \exp(-\beta E(\sigma)/Z)$$
 (3.2)

where Z is the partition function which is given by

$$Z = \sum_{\sigma} \exp(-\beta E(\sigma)) \tag{3.3}$$

The sum is over all the spin configurations on our finite volume. In our definition of H we have only included the nearest neighbor pairs such that both sites are in finite volume. This is usually called "free" boundary conditions[36]. Knowing the partition function allows us to derive different statistical quantities such as the Free energy:

$$F = -kT \ln Z \tag{3.4}$$

The average value of the spin at the origin denoted by $\langle ... \rangle$ equal to:

$$\langle \sigma_0 \rangle = \frac{1}{Z} \sum_{\sigma} \exp(-\beta E(\sigma))$$
 (3.5)

The internal energy is

$$U = \langle E \rangle$$

$$= -\frac{1}{Z} \left(\frac{\partial Z}{\partial \beta} \right)$$
(3.6)

And by using the above definitions (3.4) and (3.7) we can verify that

$$U = kT^{2} \frac{\partial}{\partial T} \ln Z$$

$$= -T^{2} \frac{\partial}{\partial T} (F/T)$$
(3.7)

Let us also denote

$$u = \frac{\partial(\beta F)}{\partial \beta} = -\frac{1}{N} \frac{\partial(\ln Z)}{\partial \beta} = -\frac{1}{NZ} \frac{\partial Z}{\partial \beta}$$

$$= -\frac{1}{NZ} \frac{\partial}{\partial \beta} \left(\sum_{(\sigma)} e^{-\beta E(\sigma)} \right) = \frac{1}{N} \left(\sum_{(\sigma)} E(\sigma) \frac{e^{-\beta E(\sigma)}}{Z} \right)$$

$$= \frac{1}{N} \langle E(\sigma) \rangle$$

$$= -J \langle \sigma_{i,j} \sigma_{i,j+1} \rangle - J' \langle \sigma_{i,j} \sigma_{i+1,j} \rangle - H \langle \sigma_{i,j} \rangle$$
(3.8)

And we consider the case where (i and j)=0

$$u = -J \langle \sigma_{0,0}\sigma_{0,1} \rangle - J' \langle \sigma_{0,0}\sigma_{1,0} \rangle - H \langle \sigma_{0,0} \rangle \tag{3.9}$$

In the absence of the magnetic field (H=0) and in isotropic case where J=J' and $\sigma_{1,0}=\sigma_{0,1}$ we can obtain the relation bellow

$$u = \frac{\partial(\beta F)}{\partial \beta} = -2J \langle \sigma_{0,0} \sigma_{0,1} \rangle \tag{3.10}$$

Using the Onsager formula for F, we obtain an expression for the correlation function $C(0,1) = \langle \sigma_{00}\sigma_{0,1} \rangle$ which it can be expressed as

$$C(0,1) = -\frac{1}{2J} \frac{\partial(\beta F)}{\partial \beta} \tag{3.11}$$

(see the Maple worksheet below).

3.3 One-Dimension Ising model

The lattice is a linear chain; we will consider the chain closed to simplify the problem with periodic boundary conditions which means we will connect the ends together to obtain a closed circle with N spins.

The Hamiltonian, with external magnetic field is:

$$E_N(\sigma_1...\sigma_N) = -J\sum_{i=1}^N \sigma_i \sigma_{i+1} - \frac{1}{2}\mu\beta \sum_{i=1}^N (\sigma_i + \sigma_{i+1})$$
 (3.12)

Where μ is the magnetic moment of the spins. We take in consideration the the infinite structure of the Ising chain, and we can rewrite the sum more symmetrical $(\sigma_{N+1} = \sigma_1)$:

3.3.1 Partition Function

In the theory of equilibrium statistical mechanics, the canonical partition function contains all the information needed to recover the thermodynamic properties of a system with fixed number of particles. We sum over the full configuration space spans over exactly 2^N states, because each spin can only have two possible values.

We will use the technique of the transfer matrices, and in order to solve the Ising Problem, we have to obtain the canonical partition function

$$Z_N = \sum_{\sigma_i} \exp \left[K \sum_{i=1}^N \sigma_i \sigma_{i+1} + \frac{L}{2} \sum_{i=1}^N (\sigma_i + \sigma_{i+1}) \right]$$
 (3.13)

 $K=\beta J$, $L=\beta\mu$, and the second term has been rearranged to take advantage of a more symmetric form. As a matter of convenience, we adopt periodic boundary conditions, $\sigma_{N+1}=\sigma_1$. There are basically two ways to work on the transfer matrix and we choose the easiest, we decompose $e^{-\beta E}$ with this previous way:

$$\begin{split} e^{-\beta E} &= e^{K\sigma_1\sigma_2 + \beta H\sigma_1} e^{K\sigma_2\sigma_3 + \beta H\sigma_2} ... e^{K\sigma_N\sigma_1 + \beta H\sigma_N} \\ &= T_{\sigma_1\sigma_2} T_{\sigma_2\sigma_3} ... T_{\sigma_N\sigma_1} \end{split}$$

where

$$T(\sigma_i \sigma_{i+1}) = \exp\left[K\sigma_i \sigma_{i+1} + \frac{L}{2}(\sigma_i + \sigma_{i+1})\right]$$
(3.14)

The sum is over all configurations of spin variables.

Transfer Matrix

We can represent with a matrix of $2x^2$ all the possible configurations of $T_{\sigma_1\sigma_2}$ with $\sigma_i = \pm 1$ [7].

$$\begin{bmatrix} T_{++} & T_{+-} \\ T_{-+} & T_{--} \end{bmatrix} = \begin{bmatrix} e^{+K+\beta H} & e^{-K+\beta H} \\ e^{-K-\beta H} & e^{+K-\beta H} \end{bmatrix}$$

And the canonical partition function is a trace of a product of N identical transfer matrices [7]

$$Z_N = Tr(T^N) (3.15)$$

Known that the transfer matrix is symmetric and can thus be diagnalized $UTU^{-1}=T$ with $U^{-1}=U^+$ and

$$UTU^{-1} = \left[\begin{array}{cc} \lambda_+ & 0 \\ 0 & \lambda_- \end{array} \right]$$

Furthermore, the canonical partition function can be written in terms of the eigenvalues of the transfer matrix

$$Z_N = Tr(UTU^{-1})^N = Tr(T)^N$$
(3.16)

and we can write

$$Z_N = Tr \left[\begin{array}{cc} \lambda_+ & 0 \\ 0 & \lambda_- \end{array} \right]^N$$

which equals to;

$$Z_N = \lambda_+^N + \lambda_-^N \tag{3.17}$$

where

$$\lambda_{\pm} = e^K \cosh(L) \mp \left(e^{2K} \cosh^2 L - 2\sinh 2K\right)^{\frac{1}{2}} \tag{3.18}$$

and they are given by the roots of the equation, $\det(T-\lambda I)=0$, and it is easy to see that these eigenvalues are always positive, and that $\lambda_1>\lambda_2$ (except at the trivial point T=0 and H=0). In zero fields, we have:

$$\lambda_{+} = 2\cosh K \ge \lambda_{-} = 2\sinh K \tag{3.19}$$

With the degeneracy $(\lambda_- = \lambda_+)$ in the limit $K \to \infty$ (that is for $T \to 0$) "it is known as the thermodynamic limit", the free energy in the thermodynamic limit is written as:

$$Z_N = \lambda_+^N \left[1 + \left(\frac{\lambda_-}{\lambda_+} \right)^N \right] \tag{3.20}$$

We are interested about the thermodynamic limits. In this limit, the free energy per site is:

$$\frac{F}{N} = \lim_{N \to \infty} \left(-\frac{1}{\beta N} \log Z_N \right) \tag{3.21}$$

$$\frac{1}{N}\log Z_N = \log \lambda_+ + \frac{1}{N}\log \left[1 + \left(\frac{\lambda_-}{\lambda_+}\right)^N\right], With \ \lambda_-/\lambda_+ < 1$$
 (3.22)

The second term decrease exponentially with N because λ_- always stay strictly smaller than λ_+ , whatever the temperature and the field applied (exception T=0, H=0):

$$g(T,H) = \frac{F}{N} = \lim_{N \to \infty} \left[\frac{-1}{N\beta} \ln Z_N \right] = -\frac{1}{\beta} \ln \lambda_+ \tag{3.23}$$

that is,

$$g(T,H) = \frac{F}{N} = -\frac{1}{\beta} ln \left\{ e^K \cosh(\beta H) + \left[e^{2K} \cosh^2(\beta H) - 2 \sinh(2K) \right]^{\frac{1}{2}} \right\}$$
(3.24)

This is an analytic function of T and H, from which we derive all the thermodynamic properties of the one-dimensional system:

$$M(T,H) = \left(\frac{\partial g}{\partial H}\right)_T = -\frac{1}{N}\frac{\partial}{\partial H}(F) = \frac{\sinh\beta H}{\left[\sinh^2\beta H + e^{-4K}\right]^{\frac{1}{2}}}$$
(3.25)

We then see that, as M(T,h=0)=0, this model is unable to explain ferromagnetism, from the entropy per spin, $s(T,h)=-(\partial g/\partial T)_H$, and we can calculate the specific heat at constant field. In zero fields, we have

$$c_{H=0} = \frac{J^2}{k_B T^2} \left[sech\left(\frac{J}{k_B T}\right) \right]^2 \tag{3.26}$$

T.'s is well-behaved function, displaying just a broad maximum as a function of temperature. We introduce easily the magnetic susceptibility in H = 0:

$$\chi = \left(\frac{\partial M}{\partial H}\right) = -\left(\frac{\partial^2 F}{\partial H^2}\right)_{H=0} = N\beta e^{2K} \tag{3.27}$$

And which stays finite in all non zero temperature; and as we've seen before all the thermo dynamical functions are regular. It can't show a singularity in finite temperature.

The Ising model in one-dimension does not possess any phase transition, at whatever the temperature

3.4 Two dimensional Ising Model

The discussion of the Onsager solution is beyond the scope of this thesis. We shall limit our consideration to a more listing of some of the Onsager results.

(coming calculation based on the work of Onsager presented by Silvio R.A Salinas)

With the thermodynamic limit with zero magnetic field and with nearest neighbor interactions, restricting the study on a square lattice. The free energy of the Ising Model can be written

$$-\beta g(T) = \ln 2 + \frac{1}{2\pi^2} \int_0^{\pi} \int_0^{\pi} \ln \left[\cosh^2 2K - \sinh 2K (\cos \theta_1 + \cos \theta_2) \right] d\theta_1 d\theta_2, \tag{3.28}$$

Where again $K = \beta J$ (in the original solution, Onsager already considered different interactions along the two directions of the square lattice [7]). Moreover, the internal energy

$$u = -\frac{J}{\tanh K} \left[1 + \frac{\sinh^2 2K - 1}{\pi^2} \times \int_0^{\pi} \int_0^{\pi} \frac{d\theta_1 d\theta_2}{\cosh^2 2K - \sinh 2K(\cos \theta_1 + \cos \theta_2)} \right]$$
(3.29)

The internal energy in this expression logarithmically diverges for

$$\cosh^2 2K = 2\sinh 2K \tag{3.30}$$

that is

$$\sinh 2K = 1\tag{3.31}$$

Which gives the Onsager critical temperature,

$$K_c^{-1} = \frac{k_B T_c}{J} = \frac{2}{\ln(1 + \sqrt{2})} = 2.269...$$
 (3.32)

In the neighborhood of the critical temperature, it is convenient to introduce a smaller parameter,

$$\delta = (\sinh 2K - 1)^2 \tag{3.33}$$

For $\delta \to 0$ we write

$$\int_{0}^{\pi} \int_{0}^{\pi} \frac{d\theta_{1}d\theta_{2}}{\cosh^{2}2K - \sinh 2K(\cos \theta_{1} + \cos \theta_{2})} \sim \int \int \frac{d\theta_{1}d\theta_{2}}{\delta + \frac{1}{2}\sinh 2K(\theta_{1}^{2} + \theta_{2}^{2})}$$

$$= 2\pi \int_{0}^{\pi} \frac{rdr}{\delta + \frac{1}{2}r^{2}\sinh 2K} \sim -2\pi \ln \delta$$
(3.34)

From this asymptotic form, we have the internal energy in the neighborhood of the critical temperature,

$$u \sim -\frac{J}{\tanh K_c} \left[1 + A(K - K_c) \ln |K - K_c| \right]$$
 (3.35)

A is a constant. By taking the derivative with respect to temperature, we get the formula of specific heat in zero fields which is

$$c_{H=0} = B \ln |K - K_c| \tag{3.36}$$

where B is a constant and $K \to K_c$.

From the pervious eq (3.31) of u, we can write an analytic expression for the internal energy in terms of an elliptic integral of the first kind

$$u = -\frac{J}{\tanh K} \left[1 + (2\tanh^2 2K - 1) \frac{2}{\pi} K(k_1) \right]$$
 (3.37)

where

$$k_1 = \frac{2\sinh 2K}{\cosh^2 2K} \tag{3.38}$$

and $K(k_1)$ is a complete elliptic integral of the first kind

$$K(k_1) = \int_0^{\pi} \left[1 - k_1^2 \sin^2 \theta \right]^{-\frac{1}{2}} d\theta \tag{3.39}$$

The specific heat can also be written in terms of complete elliptic integrals (of first and second kind). Unfortunately, however, we do not have generalizations of these results for either three dimensions or in the presence of an external magnetic field.

3.5 Duality Kramers-Wannier

Kramers and Wannier guessed the exact critical temperature of the 2D square lattice in 1941[14]. The comparison of high to low temperature expansion of the partition function. Consider a square lattice with periodic boundary conditions the partition function will be written as:

$$Z = (\cosh K)^{s} \sum_{\sigma_{i}} \prod_{\langle i,j \rangle} (1 + \tanh K \sigma_{i} \sigma_{j})$$
(3.40)

where s is the total number of first neighbors pairs $\langle i, j \rangle$.

3.5.1 High temperature expansion (HTE)

Reforming the Boltzmann factor $e^{-\beta E}$, and by expanding this latter expression the partition function can be expressed as follow:

$$Z = 2^{N} (\cosh K)^{s} f(\tanh K)$$
(3.41)

and

$$f(a) = \sum_{n} c_n a^n \tag{3.42}$$

where c_n is a coefficient which counts the number of closed loops of length n, in one-dimension

3.5.2 Low temperature expansion (LTE)

We consider the low temperature expansion on the dual lattice, we define new sites denoted by the sign σ^* , placed in the center of each mesh of the lattice [8]. These new sites σ^* constitute a new lattice which we call dual lattice.

We notice that the dual lattice has the same form as the original one which is a square lattice. and for clarification, the dual lattice of an hexagonal lattice is a triangular lattice and vice versa consider the case of square lattice. The Hamiltonian is

$$E^* = -J^* \sum_{i,j} \left(\sigma_{i-1/2,j-1/2}^* \sigma_{i-1/2,j+1/2}^* + \sigma_{i-1/2,j-1/2}^* \sigma_{i+1/2,j-1/2}^* \right)$$
(3.43)

Assuming J* is positive

3.5.3 Comparison

Kramers and Wannier argued that if the partition function or equivalently the free energy has singularity at the critical point and no other singularity, then it must be determined by [8]

$$e^{-2K_c} = \tanh K_c \tag{3.44}$$

with

$$K_c = \frac{1}{2}\ln(1+\sqrt{2}) = 0.4407$$
 (3.45)

And the same result occurs in Onsager's exact solution [15]. In this way, there is a relation between the partition function and similarly the free energy at high $(K < K_c)$ and low $(K^* > K_c)$ temperature for [8]

$$\tanh K = e^{-2K^*} \to \tanh K^* = e^{-2K} \to \sinh 2K \sinh 2K^* = 1$$
 (3.46)

The square lattice is a self-dual since the original and the dual have the same form, resulting the HTE and the LTE are preformed on the same lattice, noting that the case is different coming to triangular lattice where the HTE is performed on triangular lattice and the LTE on a honeycomb lattice and their partition functions are given respectively

$$Z_3^{HTE}(K) = 2^N (\cosh K)^s f_3(\tanh K)$$
(3.47)

$$Z_3^{LTE}(K) = 2e^{sK} f_6\left(e^{-2K}\right) \tag{3.48}$$

$$Z_6^{HTE}(K) = 2^N (\cosh K)^s f_6(\tanh K)$$
 (3.49)

$$Z_6^{LTE}(K) = 2e^{sK} f_3\left(e^{-2K}\right)$$
 (3.50)

As a result $Z_3(K)$ and $Z_6(K^*)$ are directly related for K and K^* giving in the previous equation. (check the Appendix B)

Chapter 4

Methodology and Numerical Procedure

4.1 Definition of Maple

Maple is mathematics software developed by researchers from the University of Waterloo in Canada and ETH Zurich University. It is distinguished by the power of its symbolic, numerical calculation and by the graphic representation of the results. It is a software for scientists, engineers, students with a good mathematical level.

This software does wonders in the calculation with very high precision, the resolution of real equations, imaginary, differential, integral, and so on.

4.2 Correlation function

The study of the general correlation function $\langle \sigma_{0,0}\sigma_{M,N}\rangle$ is complicated. However, there are two special cases where this correlation function possesses the simplifying feature that it may be written as a Toeplitz determinant.

1°- m=0, n arbitrary,

2°- m = n. Which is a the diagonal correlation function, and can be calculated by the Toeplitz¹ determinants,

And for more complicated case is the Quadratic recursion relations on the correlation functions when $m \neq n$.

The spin-spin correlation functions, considering thermodynamic limits:

$$\left\langle \sigma_{m',n'}, \sigma_{m,n} \right\rangle = \lim_{m \to \infty, n \to \infty} \left\langle \sigma_{m',n'} \sigma_{m,n} \right\rangle_{m,n} = \lim_{m \to \infty, n \to \infty} \frac{\sum_{\sigma} \sigma_{m',n'} \sigma_{m,n} e^{-\beta \epsilon}}{Z(\beta)}$$
(4.1)

and

$$M(H) = \lim_{m \to \infty, n \to \infty} \left\langle \frac{1}{(mn)} \sum_{j,k} \sigma_{j,k} \right\rangle_{m,n} = \lim_{m \to \infty, n \to \infty} \left\langle \sigma_{0,0} \right\rangle_{m,n} \tag{4.2}$$

In the continuous case we note that

¹ A Toeplitz determinant is the determinant of a matrix whose elements $a_{m,n}$ are functions of m-n

$$M(T,H) = \frac{\partial}{\partial H} \left(\frac{1}{N\beta} \ln Z \right) = \frac{1}{N\beta Z} \frac{\partial Z}{\partial H}$$

$$= \frac{1}{N\beta Z} \frac{\partial}{\partial} \left(\sum_{(\sigma)} e^{-\beta E(\sigma)} \right) = \frac{1}{N\beta Z} \sum_{(\sigma)} e^{-\beta E(\sigma)} \frac{\partial}{\partial H} (-\beta E(\sigma))$$

$$= -\frac{1}{N} \frac{\sum_{(\sigma)} e^{-\beta E(\sigma)}}{Z} \left(-\sum_{i,j} \sigma_{i,j} \right)$$

$$= \frac{1}{N} \left\langle \sum_{i,j} \sigma_{i,j} \right\rangle = \frac{1}{N} \left\langle N \sigma_{i,j} \right\rangle$$

and it is equal to:

$$M(T,H) = \langle \sigma_{0,0} \rangle \tag{4.3}$$

Furthermore, the spontaneous magnetization as the limit $M_0 = \lim_{H\to 0^+} M(H,T)$. Furthermore, in a lattice on m rows and n columns, we define the magnetic susceptibility per site $\chi(H)$ as [10]

$$\chi(T,H) = \frac{\partial \overline{M(H)}}{\partial H},\tag{4.4}$$

and it can be expressed also in term of spin-spin correlation function as thermodynamic limit. The susceptibility is defined as

$$\chi(T,H) = \frac{\partial M(H)}{\partial H} \tag{4.5}$$

Restricting with Onsager lattice to write the previous equation as

$$\chi(T,H) = \frac{\partial^2 \ln Z}{\partial H^2} = \frac{1}{N} \frac{\partial}{\partial H} \left(\frac{\sum_{(\sigma)} e^{-\beta E(\sigma)}}{Z} \left(\sum_{i,j} \sigma_{i,j} \right) \right)$$
(4.6)

$$= \frac{\beta}{N} \sum_{(\sigma)} \frac{\sum_{(\sigma)} e^{-\beta E(\sigma)}}{Z} \left(\sum_{k,l} \sigma_{k,l} \right) \left(\sum_{i,j} \sigma_{i,j} \right) + \frac{1}{N} \sum_{\sigma} e^{-\beta E(\sigma)} \left(\sum_{i,j} \sigma_{i,j} \right) \frac{\partial}{\partial H} \frac{1}{Z}$$
(4.7)

However,

$$\frac{\partial}{\partial H}\frac{1}{Z} = -\frac{1}{Z}\frac{\partial \ln Z}{\partial H} = -\frac{N\beta M(T, H)}{Z} \tag{4.8}$$

and,

$$\begin{split} \chi(T,H) &= \frac{\beta}{N} \sum_{(\sigma)} \frac{\sum_{(\sigma)} e^{-\beta E(\sigma)}}{Z} \left(\sum_{k,l} \sigma_{k,l} \right) \left(\sum_{i,j} \sigma_{i,j} \right) \\ &- \frac{1}{N} \sum_{\sigma} e^{-\beta E(\sigma)} \left(\sum_{i,j} \sigma_{i,j} \right) \frac{N\beta M(T,H)}{Z} \end{split}$$

Using,

$$\frac{1}{N} \sum_{(\sigma)} \frac{e^{-\beta E(\sigma)}}{Z} \left(\sum_{i,j} \sigma_{i,j} \right) = M(T, H)$$

and,

$$\sum_{(\sigma)} \frac{e^{-\beta E(\sigma)}}{Z} \left(\sum_{k,l} \sigma_{k,l} \right) \left(\sum_{i,j} \sigma_{i,j} \right) = \sum_{k,l} \sum_{i,j} \left\langle \sigma_{i,j} \sigma_{k,l} \right\rangle = N \sum_{k,l} \left\langle \sigma_{0,0} \sigma_{k,l} \right\rangle$$

we finally obtain

$$\chi(T,H) = \beta \sum_{k,l} \left\langle \sigma_{0,0} \sigma_{k,l} \right\rangle - N\beta M^{2}(T,H)$$

$$= \beta \sum_{k,l} \left(\left\langle \sigma_{0,0} \sigma_{k,l} - M^{2}(T,H) \right\rangle \right)$$
(4.9)

When $H \to 0^+$, the zero-field magnetic susceptibility $\chi(T,0)$ can be written in terms of the spin-spin correlation functions $C(M,N) = \langle \sigma_{0,0}\sigma_{k,l} \rangle$ as

$$\chi(T,H) = \beta \sum_{k,l} \left\langle \sigma_{0,0} \sigma_{k,l} \right\rangle - M_0^2$$

$$= \beta \sum_{M=-\infty}^{+\infty} \sum_{N=-\infty}^{+\infty} \left(C(M,N) - M_0^2 \right)$$
(4.10)

where N and M representing rows and columns respectively (the total numbe of sites is then $\aleph = MN$).

The spontaneous magnetization is obtained as the limiting value of an infinite Toeplitz determinant when $T < T_c$. Where T_c is the critical temperature.

$$D_{i} = \begin{bmatrix} a_{0} & a_{-1} & a_{-2} & \dots & a_{-i+1} \\ a_{1} & a_{0} & a_{-1} & \dots & a_{-i+2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{i-1} & a_{i-2} & a_{i-3} & \dots & a_{0} \end{bmatrix}$$

$$(4.11)$$

Where

$$a_{n'} = \frac{1}{2\pi} \int_0^{2\pi} d\theta e^{-in'\theta} \Phi(\theta)$$
 (4.12)

Where $\Phi(\theta)$ is the weight distribution and it equal to:

$$\Phi(\theta) = \left[\frac{(1 - \alpha_1 e^{i\theta})(1 - \alpha_2 e^{-i\theta})}{(1 - \alpha_1 e^{-i\theta})(1 - \alpha_2 e^{+i\theta})} \right]^{1/2}$$
(4.13)

Where for $\langle \sigma_{0,0}, \sigma_{N,N} \rangle$

$$\Phi(\theta) = \left[\frac{\sinh 2\beta E_1 \sinh 2\beta E_2 - e^{-i\theta}}{\sinh 2\beta E_1 \sinh 2\beta E_2 - e^{i\theta}} \right]^{1/2}$$
(4.14)

$$\alpha_1 \to 0$$
 $\alpha_2 \to (\sinh 2\beta E_1 \sinh 2\beta E_2)^{-1}$ (4.15)

for $\langle \sigma_{0,0}, \sigma_{0,N} \rangle$

$$\alpha_1 = e^{-2E_1/k_B T} \cdot \tanh E_2/k_B T$$
 $\alpha_2 = e^{-2E_1/k_B T} \coth E_2/k_B T$
(4.16)

4.3 Correlation function C(0,1)

"Near-neighbor Correlation functions" From the eq (4.18)the integral (4.17) and by replacing N by 1 we find:

$$\langle \sigma_{0,0}, \sigma_{0,1} \rangle = \frac{1}{2\pi} \int_0^{2\pi} d\theta \left[\frac{(1 - \alpha_1 e^{i\theta})(1 - \alpha_2 e^{-i\theta})}{(1 - \alpha_1 e^{-i\theta})(1 - \alpha_2 e^{+i\theta})} \right]^{1/2}$$
(4.17)

Which returns to (check the calculation done bellow by Maple)

$$C(0,1):=1/2*(1+k)^{(1/2)}*(k-1)*K/k^{(1/2)}+1/2*(1+k)^{(1/2)}/k^{(1/2)}$$

$$Ct(0,1) := -1/2*(k-1)*(1+k)^(1/2)*K+1/2*(1+k)^(1/2):$$

(4.18)

Example

From the matrix (4.16) above we can write

$$C(0,0) = a_0$$

$$C(1,1) = \begin{bmatrix} a_0 & a_{-1} \\ a_1 & a_0 \end{bmatrix} = a_0^2 - a_1 a_{-1}$$

4.4 Method

4.4.1 The Onsager solution

the free energy per site as $-f/kT=-\beta f=F$ is given by ([eq (15.133), Kerson, Huang] [3] the following integral,see(3.30))

what we are trying to do here is to express the following integral in term of k and t

$$mbf = \ln AA + \int_0^{\pi} \frac{1}{2} \frac{\ln\left(\frac{1}{2} + \frac{1}{2}\sqrt{1 - BB^2 \sin^2(\omega)}\right)}{\pi} d\omega$$
 (4.19)

where we have

$$BB = \frac{2}{\cosh(2\beta J)\cosh(2\beta J)} \tag{4.20}$$

and also we have

$$AA = 2\cosh(2\beta J) \tag{4.21}$$

we recall that

$$\beta = \frac{1}{k_B T}$$

defining

$$k = \frac{1}{\sinh(2\beta J)^2} \tag{4.22}$$

so to that point we can define BB and AA in terms of k as so

$$BB = \frac{2\sqrt{k}}{k+1} \tag{4.23}$$

33

which is the Landen transform of k. now for AA the same prosses

$$AA = \frac{2\sqrt{k(k+1)}}{k} \tag{4.24}$$

and now we replace the previous esults in the expression of mbf

$$mmbf = \ln\left(\frac{2\sqrt{k(k+1)}}{k}\right) + \int_0^{\pi} \frac{1}{2} \frac{\ln\left(\frac{1}{2} + \frac{1}{2}\sqrt{1 - \frac{4k\sin(\omega)^2}{(k+1)^2}}\right)}{\pi} d\omega \tag{4.25}$$

The expression of the correlation function C(0,1)

Our aim now is to calculate C(0,1) once the Onsager solution of the free energy (mbf = -beta * f) is known.

We will use the expression above with an integral on omega.

$$C(0,1) = \frac{1}{2} \frac{\frac{d}{d\beta} MBF(\beta)}{J}$$

$$(4.26)$$

and since we know hat it exist a relation between k and β . where in low temperature regime k < 1 and $T < T_c = \frac{2J}{\ln(1+2^{1/2})k}$ So

$$C(0,1) = \frac{1}{2} \frac{\left(\frac{d}{dk} MBF(k)\right) \left(\frac{d}{d\beta} k(\beta)\right)}{J}$$
(4.27)

One can easily establish from the definition of k that

$$\frac{1}{2} \frac{\frac{d}{d\beta} k(\beta)}{J} = -2k^{3/2} \sqrt{\frac{k+1}{k}}$$
 (4.28)

so replacing the equation above in C(0,1) we find

$$C(0,1) = -2k^{3/2}\sqrt{\frac{k+1}{k}} \left(\frac{d}{dk} MBF(k)\right)$$
(4.29)

Now replace MBF(k) by Onsager solution

$$mmbf = \frac{1}{2} \ln \left(\frac{2(k+1)}{k} \right) + \int_0^{\frac{\pi}{2}} \frac{\ln \left(1 + \sqrt{1 - \frac{4k \sin(\omega)^2}{(k+1)^2}} \right)}{\pi} d\omega$$
 (4.30)

Let us calculate the derivative d/dk(mmbf) appearing in C01 the first gives

$$T_1 = -\frac{1}{2k(k+1)} \tag{4.31}$$

Finally, introducing kL (kL = 2 * sqrt(k)/(1+k) which is called the Landen transform of k)

$$k_L = \frac{2\sqrt{k}}{k+1} \tag{4.32}$$

the result will be

$$\frac{2\sin(\omega)^2(k-1)}{\sqrt{1-k_L^2\sin(\omega)^2}\left(1-k_L^2\sin(\omega)^2\right)}\tag{4.33}$$

we integrate the previous expression to ω and we find

$$T_2 = -\frac{1}{4} \frac{(k+1)\left(\pi - 2EllipticK\left(\frac{2\sqrt{k}}{k+1}\right)\right)}{(k+1)\pi k}$$

$$\tag{4.34}$$

Conclusion, C01 is the sum of T1 and T2

$$C(0,1) = -2\sqrt{\frac{k+1}{k}}k^{3/2}\left(-\frac{1}{2k(k+1)} - \frac{1}{4}\frac{(k-1)(\pi - 2EllipticK(\frac{2\sqrt{k}}{k+1})}{(k+1)\pi k}\right)$$
(4.35)

We can write this result in a different form using the identity on the *Elliptic* functions

$$EllipticK\left(\frac{2\sqrt{k}}{k+1}\right) = (k+1)EllipticK(k)$$
(4.36)

and now by replacing the correlation function C(0,1)

$$CC01 = -2\sqrt{\frac{k+1}{k}}k^{3/2}\left(-\frac{1}{2k(k+1)} - \frac{1}{4}\frac{(k-1)(\pi - 2(k+1)EllipticK(k))}{(k+1)\pi k}\right)$$
(4.37)

We have now two equivalent expressions for C(0,1)

$$CC01 = -\frac{\frac{k+1}{k}\sqrt{k}(k-1)EllipticK\left(\frac{2\sqrt{k}}{k+1}\right)}{(k+1)\pi} + \frac{\sqrt{\frac{k+1}{k}}\sqrt{k}}{2}$$

$$cC01 = -\frac{EllipticK(k)(k-1)\sqrt{k}\sqrt{\frac{k+1}{k}}}{\pi} + \frac{\sqrt{\frac{k+1}{k}}\sqrt{k}}{2}$$

$$(4.38)$$

after some simplifications, the two equivalent expressions are

$$sC01 = \frac{(-k+1)EllipticK\left(\frac{2\sqrt{k}}{k+1}\right)}{\sqrt{k+1}\pi} + \frac{\sqrt{k+1}}{2}$$

$$sCC01 = \frac{\sqrt{k+1}(-k+1)EllipticK(k)}{\pi} + \frac{\sqrt{k+1}}{2}$$

$$(4.39)$$

Let show the plot of C01 in terms of k, for $k \in [0, \infty]$, For comparison, we have also plotted the function $(1-k^2)^{1/4}$ which is the square of the spontaneous magnetization $(1-k^2)^{1/8}$ (Yang result)

$$sC01 = \frac{(-k+1)EllipticK\left(\frac{2\sqrt{k}}{k+1}\right)}{\sqrt{k+1}\pi} + \frac{\sqrt{k+1}}{2}$$

$$\chi = \frac{M}{H} \quad (IS) \quad \chi = \frac{\mu_0 M}{H}$$

$$(4.40)$$

Important remark

The plot with the second expression is more "problematic", only the part k < 1 is plotted !!! The reason is that the EllipticK(k) function is well defined (has a convergent series) only if k < 1

$$sCC01 = \frac{\sqrt{k+1}(-k+1)EllipticK(k)}{\pi} + \frac{\sqrt{k+1}}{2}$$

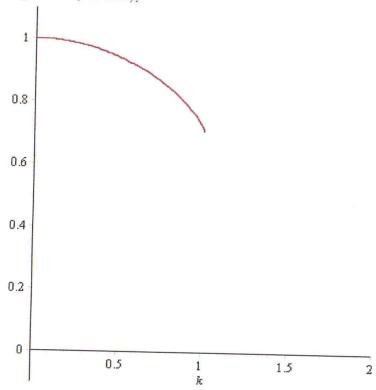
$$(4.41)$$

4.4. METHOD 35

$$sCCOI := (k+1)^{(1/2)*(-k+1)/Pi*EllipticK(k) + 1/2*(k+1)^{(1/2)};$$

$$sCCO1 := \frac{\sqrt{k+1} (-k+1) \text{ Elliptic} K(k)}{\pi} + \frac{1}{2} \sqrt{k+1}$$

plot([sCC01], k=0..2,-.1..1.1);



So how to deal with the other part k > 1?

One has to use the following observation.. Let us recall the identity

$$EllipticK\left(\frac{2\sqrt{k}}{k+1}\right) = (k+1)EllipticK(k) \tag{4.42}$$

since the left side is invariant under k->1/k, the last identity can also be written as

$$EllipticK\left(\frac{2\sqrt{k}}{k+1}\right) = \left(1 + \frac{1}{k}\right)EllipticK\left(\frac{1}{k}\right) \tag{4.43}$$

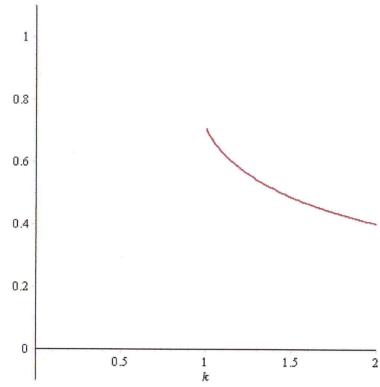
and then, when comparing the two last identities, one has for any \boldsymbol{k}

$$(k+1)EllipticK(k) = \left(1 + \frac{1}{k}\right)EllipticK\left(\frac{1}{k}\right)$$
(4.44)

So a third possibility for writing C01 is

$$ssCC01 = \frac{\sqrt{k+1}(-k+1)Elliptic\left(\frac{1}{k}\right)}{\pi k} + \frac{k+1}{2}$$
(4.45)

Plotting this new function, we see that we obtain the other part of the plot. EllipticK(1/k) is now well defined for 1/k < 1, i.e. for k > 1 !!! plot([ssCC01], k=0..2,-.1..1.1);



Putting these two plots together, we obtain he desired plot for all values of k ($k \in [0, \infty]$) with(plots):

1.5

Graph1 := plot([sCC01], k= 0 .2,-.1 ..1.1) : Graph2 := plot([ssCC01], k= 0 ..2,-.1 ..1.1) : display(Graph1, Graph2);

> 0.8 0.6 0.4 0.2

0.5

Important: These remarks for C(0,1) are valid for any C(M,N)

$$sCC01 = \frac{\sqrt{k+1}(-k+1)EllipticK(k)}{\pi} + \frac{\sqrt{k+1}}{2}$$

which well defined for k < 1, is called the low temperature C(0,1) correlation function, written C < (0,1)

$$ssCC01 = \frac{\sqrt{k+1}(-k+1)Elliptic\left(\frac{1}{k}\right)}{\pi k} + \frac{k+1}{2}$$

which well defined for k > 1, is called the high temperature C(0,1) correlation function, written C > (0,1)

Now if we perform the transformation k->1/k, on these two correlations, we obtain what is called dual correlations

$$dCC01 = \frac{\sqrt{1+1/k}(1-1/k)EllipticK(1/k)}{\pi} + \frac{\sqrt{1+1/k}}{2}$$
(4.46)

which well defined for k > 1, is called the high temperature Cd(0,1) dual correlation function, written Cd > (0,1)

$$ddCC01 = \frac{\sqrt{1 + 1/k}(1 - 1/k)EllipticK(k)k}{\pi} + \frac{\sqrt{1 + 1/k}}{2}$$
(4.47)

which well defined for k < 1, is called the low temperature Cd(0,1) dual correlation function, written Cd < (0,1).

4.5 Diagonal Correlation functions C(N,N)

The diagonal spin-spin correlation functions of the square Ising model C(N, N), and it's dual $C_t(N, N)$, can be calculated from Toeplitz determinants:

$$C(N,N) = \det(a_{i-j})$$
 $1 \le i, j \ge n$
$$C_t(N,N) = (-1)^n \cdot \det(a_{i-j-1}) \quad 1 \le i, j \ge n$$
 (4.48)

And we introduce the elements a_N in term of hypergeometric function for $N \leq -1$

$$a_{N} = -\frac{\left(-\frac{1}{2}\right)_{N+1}}{(N+1)!} * t^{\frac{N}{2}+1/2} * {}_{2}F_{1}(1/2, N+1/2; N+2; t)$$

$$(4.49)$$

And for $N \leq -1$

$$a_{N} = -\frac{\left(-\frac{1}{2}\right)_{-N-1}}{(-N-1)!} * t^{-\frac{N}{2}-1/2} * {}_{2}F_{1}(-1/2, -N-1/2; -N; t)$$

$$(4.50)$$

Where $t = k^2 = s^4$, s^2 is defined as an elliptic modulus $k = \sinh 2K = k_>$ [19] where $K = \beta J$ and is <1 for $T > T_c$ and >1 for $T < T_c$ with $k \to (1/k) \equiv k_<$ and which gives the Kramers-Wannier duality transformation[20].

 F_1 Is a hypergeometric functions which are both including complete elliptic functions E and K.

$$\{E = 2/Pi*Elliptic E(k), K = 2/Pi*Elliptic K(k)$$

$$(4.51)$$

Example

for example the expression of $a_4 = -\frac{7}{265}k^{5/2}F_1\left(\left[\frac{1}{2},\frac{9}{2}\right],[6],k^2\right)$ can be written:

>
$$a(4) := \frac{\text{pochhammer}\left(-\frac{1}{2}, 5\right)}{5!} \cdot k^{\frac{5}{2}} \cdot \text{hypergeom}\left(\left[\frac{1}{2}, \frac{9}{2}\right], [6], k^2\right);$$

 $a(4) := -\frac{7}{256} k^{5/2} \text{hypergeom}\left(\left[\frac{1}{2}, \frac{9}{2}\right], [6], k^2\right)$

 α_N is Pochhammer symbol.

(check the Appendix A about the calculations of a_n)

Remark:

The quantities a_N are calculated by Maple as we will explain in the coming See the Program

4.6 Quadratic recursion relations on the correlation functions C(M,N)

Recursion relations relate the high-temperature correlation functions C(M, N) when $T > T_C$ to the dual correlation Ct(M, N) when $T < T_c$. The Quadratic difference equations for the spin-spin correlation function or Perk recursions [21] [20]

$$k.[c(M,N)^2 - c(M,N-1).c(M,N+1)] + [ct(M,N)^2 - ct(M-1,N).ct(M+1,N)] = 0 \quad (4.52)$$

$$k.[ct(M,N)^2-ct(M-1,N).c(M+1,N)]+[c(M,N)^2-c(M,N-1).c(M,N+1)]=0 \quad (4.53)$$

$$k.[ct(M,N).ct(M+1,N+1) - c(M,N+1).ct(M+1,N)] - c(M,N).c(M+1,N+1) + c(M,N+1).c(M+1,N) = 0$$

$$(4.54)$$

Which hold for all m and n except M = 0, N = 0, that we can rewrite:

$$C(0,1) = (1+k)^{1/2} - \sqrt{k} \cdot Ct(0,1)$$
(4.55)

With,

$$C(0,0) = Ct(0,0) = 1$$

$$C(m,n) = C(n,m) = C(|m|,|n|),$$

$$Ct(m,n) = Ct(n,m) = Ct(|m|,|n|).$$
(4.56)

We will use the previous result of the diagonal correlation function C(N, N) and its dual as inputs, and we variants the m and n, and by solving the equation to the zero we can Eventually get a correlation function C(M, N)

4.7 work done in Maple Worksheets

recrusion of Perk

$$\begin{aligned} eq1 &:= k \sim \left(c(m,n)^2 - c(m,|n-1|) \ c(m,n+1)\right) + ct(m,n)^2 - ct(|m-1|,n) \ ct(m+1,n) \\ eq2 &:= k \sim \left(c(m,n)^2 - c(|m-1|,n) \ c(m+1,n)\right) + ct(m,n)^2 - ct(m,|n-1|) \ ct(m,n+1) \\ eq3 &:= k \sim \left(c(m,n) \ c(m+1,n+1) - c(m,n+1) \ c(m+1,n)\right) - ct(m,n) \ ct(m+1,n+1) \\ &+ ct(m,n+1) \ ct(m+1,n) \end{aligned}$$

Input

```
C(0,0):=1:
         Ct(0,0):=1:
        C(0,1):=1/2*(1+k)^{(1/2)}*(k-1)*K/k^{(1/2)}+1/2*(1+k)^{(1/2)}/k^{(1/2)}:
        Ct(0,1):=-1/2*(k-1)*(1+k)^(1/2)*K+1/2*(1+k)^(1/2):
       C(1,1):=1/k*E+K*(k-1)*(1+k)/k:
       Ct(1,1):=E:
       \texttt{C(2,2)} := -1/3 * (-5 + k^2)/k^2 * \texttt{E^2+8/3} * (k-1) * (1+k) * \texttt{K*E/k^2+(k-1)^2} * (1+k)^2 * \texttt{K^2/k^2} : \\  = -1/3 * (-5 + k^2)/k^2 * \texttt{E^2+8/3} * (k-1) * (1+k) * \texttt{K*E/k^2+(k-1)^2} * (1+k)^2 * \texttt{K^2/k^2} : \\  = -1/3 * (-5 + k^2)/k^2 * \texttt{E^2+8/3} * (k-1) * (1+k) * \texttt{K*E/k^2+(k-1)^2} * (1+k)^2 * \texttt{K^2/k^2} : \\  = -1/3 * (-5 + k^2)/k^2 * \texttt{E^2+8/3} * (k-1) * (1+k) * \texttt{K*E/k^2+(k-1)^2} * (1+k)^2 * \texttt{E^2+8/3} * (1+k)^2 * \texttt{E^2+8
      \texttt{Ct}(2,2) := 1/3 * (5*k^2-1)/k^2 * E^2 + 2/3 * (k-1)^2 * (1+k)^2 * K*E/k^2 - 1/3 * (k-1)^2 * (1+k)^2 * K^2/k^2 : 1/3 * (k-1)^2 * (1+k)^2 * (1+k
 we solve by recrussion
  eq1(m=0, n=1) donne C(0,2)
              eq2(m=0, n=1) donne Ct(0,2)
              eq1(m=1, n=1) - eq3(m=0, n=1) donne C(1,2)
              eq1(m=1, n=1) + eq3(m=0, n=1) donne Ct(1,2)
eq1(m=0, n=2) donne C(0,3)
      eq2(m=0, n=2) donne Ct(0,3)
      eq1(m=1, n=2) donne C(1,3)
      eq2(m=1, n=2) donne Ct(1,3)
    eq1(m=2, n=2) - eq3(m=1, n=2) donne C(2,3)
    eq1(m=2, n=2) + eq3(m=1, n=2) donne Ct(2,3)
    eq1(m=0, n=3) donne C(0,4)
   eq2(m=0, n=3) donne Ct(0,4)
  eq1(m=1, n=3) donne C(1,4)
  eq2(m=1, n=3) donne Ct(1,4)
 eq1(m=2, n=3) donne C(2,4)
 eq2(m=2, n=3) donne Ct(2,4)
 eq1(m=3, n=3) - eq3(m=2, n=3) donne C(3,4)
 eq1(m=3, n=3) + eq3(m=2, n=3) donne C(3,4)
 These dates date dates date dates da
etc.
```

Conclusion

The phenomenon of ferromagnetism emerges when a collection of particle spins align such that their associated magnetic moments all point in the same direction, yielding a macroscopic sized net magnetic moment.

The simplest theoretical description of ferromagnetism was given by the Ising model which was invented by Wilhelm Lenz in 1920 and named after his student Ernst Ising who introduced it in his PhD thesis in 1925.

Ising has introduced his model by supposing nearest-neighbor interactions between spins on a lattice and an interaction with an external magnetic field H.

Using statistical physics methods, the model has been solved exactly in one dimension (for any H) and in two dimensions (for H=0) and the corresponding free energy and spontaneous magnetization have been obtained in terms of the temperature. In two dimensions, it can be seen that this model can describe and explain phase transition phenomena.

We studied in this thesis some of the properties of this model, among them the magnetic susceptibility and their associated correlations functions.

In the first chapter, we briefly gave a general idea about the position of the model in thermodynamic physics by explaining some approximation methods as well as some concepts that the model is concerned about in particular the important physical concept of phase transition.

In the second chapter where we introduced the whole concept of magnetization and its appearance in nature. We discussed the different types of magnetic materials as well as their proprieties and most importantly the ferromagnetism phase.

In the third chapter, we introduced the Ising model almost generally recalling its historical background, then we gave its general definition and explained its simple concept. We then introduced the solution that Ising obtained in one dimension using the transfer matrix method. We then discussed the exact solution of Onsager that he obtained for a two-dimensional model.

This exact solution has been used as a starting point for our calculations in the next chapter where another quantity of physical interest for the model, which is the magnetic susceptibility, and which has been widely investigated in the last decades by many authors. This quantity has still no clear analytical status, however, we know that it can be expressed as an infinite sum of spin correlation functions.

In the fourth chapter, we presented a useful algorithm, using quadratic recursion relations, which allows the calculations of the analytical expressions of these correlation functions C(M, N) in terms of the temperature for all values of M and N in the isotopic case (J = J') when the magnetic field is zero (H = 0).

The method on how to calculate the different correlation functions C(M,N) according to their M and N values is the following. For the diagonal correlation functions C(M,M) we used a Teoplitz determinant relation. The elements a(N) of these determinants are expressed in terms of hypergeometrical functions. Finally, a quadratic recursion relation is used to obtain

the remaining non diagonal expressions $\mathcal{C}(M,N)$, with M different of N.

There are many perspectives for future related works, let us mention only two, firstly, that this algorithm can be extended to the anisotropic case (when J is not equal to J'), and secondly, that one can analyse easily the singular behavior near the critical temperature point from the expressions that we have obtained.

Let also note that we have widely used the Maple software as a useful mathematical tool for numerical and formal calcutions in order to obtain these exact results.

Appendix A

with(gfun);

The Help gives the following information:

The gfun Package

Calling Sequence

Function (args)

gfun[function](args)

• Description:

The gfun package has been designed as a help for the manipulation and discovery of functions or sequences satisfying linear differential or recurrence equations.

with(DEtools);

Calling Sequence

DEtools[command](arguments)

Command (arguments)

• Description:

The DEtools package contains commands that help working with differential equations.

• Envdiffopdomain := [Dx, x]:

The argument domain describes the differential algebra. If this argument is the list [Dx, x] then the differential operators are notated with the symbols Dx and x. They are viewed as elements of the differential algebra C(x)[Dx] where C is the field of constants, and Dx refers to the differentiation operator d/dx.

```
\begin{aligned} hole &\coloneqq \mathbf{proc}(F) \\ &\mathbf{local}\,A: \\ A &\coloneqq de2diffop(holexprtodiffeq(F,y(x))[1],y(x)): \\ &\mathbf{return}\,collect(A/coeff(A,Dx,degree(A,Dx)),Dx,factor): \\ &\mathbf{end}\,\mathbf{proc}: \end{aligned}
```

The previous procedure hole (F(x)) make it possible to find the operator whose is solution or in other words to find the operator that cancels the function ;which is a generator operator By definition

$$\begin{aligned} aq &:= n \to \text{if } (n \ge -1) \text{ then} \\ & \text{pochhammer} (-1/2, n+1)/(n+1)! \cdot x^{(2\cdot n+2)} \cdot \text{hypergeom} ([1/2, n+1/2], [n+2], x \\ & ^4); \\ & \text{else} \\ & \text{pochhammer} (1/2, -n-1)/(-n-1)! \cdot x^{(-2\cdot n-2)} \cdot \text{hypergeom} ([-1/2, -n-1/2], [-n], x^4); \\ & \text{fi:} \end{aligned}$$

objective of the calculations that follow is to find the expressions of the aq(ii) in the form

$$aq(ii) := \frac{2P(x) \text{ EllipticK}(x^2)}{\pi} + \frac{2Q(x) \text{ EllipticE}(x^2)}{\pi}$$

gfun[holexprtodiffeq] - produce a differential equation satisfied by a holonomic expression.

Calling Sequence:

holexprtodiffeq(expr, y(z))

Parameters:

expr - holonomic expression in y(z)

y, z - name of the holonomic function and the generic variable

If expr is a holonomic expression, then gfun[holexprtodiffeq] returns a differential equation in y and z that is satisfied by expr. Initial conditions are given whenever possible.

Not all holonomic functions are recognized by holexprtodiffeq.

Example

$$Lk := hole \left(\text{hypergeom} \left(\left[\frac{1}{2}, \frac{1}{2} \right], [1], x^4 \right) \right)$$

$$Lk := Dx^2 + \frac{\left(5x^4 - 1 \right) Dx}{x \left(x - 1 \right) \left(x + 1 \right) \left(x^2 + 1 \right)} + \frac{4x^2}{\left(x - 1 \right) \left(x + 1 \right) \left(x^2 + 1 \right)}$$

We are looking to calculate a(5), which means aq(5)

$$ii := 5$$

 \rightarrow L0 := hole(aq(ii));

$$L0 := Dx^2 + \frac{Dx}{x} - \frac{4(5x^2 - 6)(5x^2 + 6)}{x^2(x - 1)(x + 1)(x^2 + 1)}$$

 ${\rm L0}$ is the operator which associate to the solution of ${\rm aq(ii)}$:

 $> R\theta := Homomorphisms(LE, L\theta)[1];$

$$\frac{1}{128} \frac{1}{x^{11}} ((x+1)(x-1)(x^2+1)(128x^{20}+120x^{16}+139x^{12}+194x^8+384x^4$$
$$-1280) Dx) + \frac{1}{64} \frac{128x^{20}+56x^{16}+71x^{12}+113x^8+272x^4-640}{x^8}$$

The Homomorphisms command finds a link between the LE and L0 operator

The Help gives the following information

DEtools [Homomorphisms] - compute the homomorphisms between two solution spaces

• Calling Sequence

Homomorphisms (L1, L2, domain)

parameters

L1 - differential operator

L2 - differential operator

domain - list containing two names

• Description

The input L1, L2 are differential operators. Denote V(L1) and V(L2) as the solution spaces of these two operators. If a map from V(L1) to V(L2) can be given in the form of a differential operator, then we call that map a homomorphism from V(L1) to V(L2). The command Homomorphisms computes a basis (as vector space) of all such homomorphisms, that is, it computes a basis of all operators r for which r(V(L1)) is a subset of V(L2).

The argument domain describes the differential algebra. If this argument is the list [Dt,t] then the differential operators are notated with the symbols Dt and t. They are viewed as elements of the differential algebra C(t)[Dt] where C is the field of constants, and Dt refers to the differentiation operator d/dt.

Result: Since E is LE solution, the relation Means that R0 (E) is a solution of L0

> $SOL := Q(ii) \cdot eval(subs(f(x) = 2/Pi \cdot EllipticK(x^2), diffop2de(R0, f(x))));$

$$SOL := Q(5) \left(\frac{1}{32} \frac{\left(128x^{20} + 56x^{16} + 71x^{12} + 113x^8 + 272x^4 - 640\right) \text{ EllipticK}(x^2)}{x^8 \pi} + \frac{1}{32} \frac{1}{x^{10} \pi} \left((x+1)(x-1)(x^2+1) \left(128x^{20} + 120x^{16} + 139x^{12} + 194x^8 + 384x^4 - 1280\right) \left(\frac{\text{EllipticE}(x^2)}{\left(-x^4 + 1\right)x^2} - \frac{\text{EllipticK}(x^2)}{x^2} \right) \right) \right)$$

> SS = series(SOL-aq(ii), x, 4*(abs(ii) + 10));

$$SS := \left(\frac{72765}{65536} Q(5) + \frac{21}{1024}\right) x^{12} + \left(\frac{114345}{262144} Q(5) + \frac{33}{4096}\right) x^{16} + \left(\frac{4459455}{16777216} Q(5) + \frac{1287}{262144}\right) x^{20} + \left(\frac{12387375}{67108864} Q(5) + \frac{3575}{1048576}\right) x^{24} + \left(\frac{294819525}{2147483648} Q(5) + \frac{85085}{33554432}\right) x^{28} + \left(\frac{916620705}{8589934592} Q(5) + \frac{264537}{134217728}\right) x^{32} + \left(\frac{23526598095}{274877906944} Q(5) + \frac{6789783}{4294967296}\right) x^{36} + \left(\frac{77301679455}{1099511627776} Q(5) + \frac{22309287}{17179869184}\right) x^{40} + \left(\frac{4141161399375}{70368744177664} Q(5) + \frac{1195140375}{1099511627776}\right) x^{44} + O(x^{48})$$

we take the smallest degree of freedom

> dd := ldegree(convert(SS, polynom), x);

$$dd := 12$$

And we solve the correspondent term to dd to 0 Note: it works for all other terms

And our purpose to find Q(ii)

> $SOLU := solve(coeff(SS, x, dd), \{Q(ii)\});$

$$SOLU := \left\{ Q(5) = -\frac{64}{3465} \right\}$$

We fix the value of Q(ii) by using the Command assign

> assign(SOLU):

We replace the pervious value in the equation Sol to find a(ii)

 $AA(ii) := map(factor, collect(map(simplify, subs(x = sqrt(k), subs({EllipticK(x^2) = Pi/2*K, EllipticE(x^2) = Pi/2*E}, SOL))), [E, K], distributed));$

$$AA(5) := \frac{1}{3465} \frac{\left(128k^{10} + 120k^8 + 139k^6 + 194k^4 + 384k^2 - 1280\right)E}{k^6}$$
$$-\frac{2}{3465} \frac{(k-1)(k+1)\left(32k^8 + 58k^6 + 87k^4 + 128k^2 + 640\right)K}{k^6}$$

> a(ii) := map(factor, collect(map(simplify, expand(AA(ii))), [E, K], distributed));

$$a(5) := \frac{1}{3465} \frac{\left(128 k^{10} + 120 k^8 + 139 k^6 + 194 k^4 + 384 k^2 - 1280\right) E}{k^6}$$
$$-\frac{2}{3465} \frac{(k-1)(k+1)\left(32 k^8 + 58 k^6 + 87 k^4 + 128 k^2 + 640\right) K}{k^6}$$

> a(-4);

```
section.
                    First a(n) functions
    > a(0);
                                                \frac{E}{k} + \frac{(k-1)(k+1)K}{k}
    > a(1);
                                        -\frac{(-2+k^2)E}{3k^2} + \frac{2(k-1)(k+1)K}{3k^2}
    > a(2);
                               -\frac{(-8+3k^2+2k^4)E}{15k^3}+\frac{(k-1)(k+1)(k^2+8)K}{15k^3}
    > a(3);
                     -\frac{\left(-48+16\,k^{2}+9\,k^{4}+8\,k^{6}\right)E}{105\,k^{4}}+\frac{4\left(k-1\right)\left(k+1\right)\left(k^{4}+2\,k^{2}+12\right)K}{105\,k^{4}}
    > a(4);
        -\frac{\left(-128+40\,k^{2}+21\,k^{4}+16\,k^{6}+16\,k^{8}\right)E}{315\,k^{5}}+\frac{\left(k-1\right)\left(k+1\right)\left(8\,k^{6}+15\,k^{4}+24\,k^{2}+128\right)K}{315\,k^{5}}
    > a(5);
      (-1280 + 384 k^2 + 194 k^4 + 139 k^6 + 120 k^8 + 128 k^{10}) E
         +\frac{2(k-1)(k+1)(32k^8+58k^6+87k^4+128k^2+640)K}{3465k^6}
    > a(6);
     -\frac{(1529 k^6 + 4480 k^2 + 1246 k^8 - 15360 + 1280 k^{12} + 2208 k^4 + 1152 k^{10}) E}{2}
          +\frac{(k-1)(k+1)(640 k^{10} + 1136 k^8 + 1647 k^6 + 2272 k^4 + 3200 k^2 + 15360) K}{45045 k^7}
   > a(-1);
                                                            -E
                                       -\frac{(-1+2k^2)E}{3k} + \frac{(k-1)(k+1)K}{3k}
                          -\frac{(-2-3k^2+8k^4)E}{15k^2}+\frac{2(k-1)(k+1)(2k^2+1)K}{15k^2}
```

```
-\frac{(-8-9 k^2-16 k^4+48 k^6) E}{105 k^3}+\frac{(k-1) (k+1) (24 k^4+13 k^2+8) K}{105 k^3}
          -\frac{(-16-16\,k^2-21\,k^4-40\,k^6+128\,k^8)\,E}{315\,k^4}+\frac{4\,(k-1)\,(k+1)\,(16\,k^6+9\,k^4+6\,k^2+4)\,K}{315\,k^4}
      \frac{(-128 - 120 k^2 - 139 k^4 - 194 k^6 - 384 k^8 + 1280 k^{10}) E}{3465 k^5}
         +\frac{(k-1)(k+1)(640 k^8 + 368 k^6 + 255 k^4 + 184 k^2 + 128) K}{3465 k^5}
 [ >
 [>
  Diagonal correlation functions
  > Ct(0,0);
   > Ct(1,1);
  > Ct(2,2);
                             \frac{(5k^2-1)E^2}{3k^2} + \frac{2(k-1)^2(k+1)^2KE}{3k^2} - \frac{(k-1)^2(k+1)^2K^2}{3k^2}
 > Ct(3,3);
    \frac{4 \left(21 \, k^2+k^6+10-96 \, k^4\right) E^3}{135 \, k^4}+\frac{4 \left(3 \, k^2+1\right) \left(k-1\right)^2 \left(k+1\right)^2 K \, E^2}{5 \, k^4}
        +\frac{8 (3 k^{4}-7 k^{2}-4) (k-1)^{2} (k+1)^{2} K^{2} E}{45 k^{4}}-\frac{4 (9 k^{2}+7) (k-1)^{3} (k+1)^{3} K^{3}}{125 k^{4}}
 > Ct(4,4);
     16 \left(1549 \, k^2 - 21773 \, k^8 + 549 \, k^{10} - 3 + 1977 \, k^4 + 5366 \, k^6 + 47 \, k^{12}\right) E^4
        -\frac{64 \left(3 k^{10}+62 k^{8}-7047 k^{6}-2997 k^{4}-1288 k^{2}+3\right) \left(k-1\right)^{2} \left(k+1\right)^{2} K E^{3}}{70875 k^{8}}
        +\frac{32 \left(3 \, k^{10}+2149 \, k^{8}-2804 \, k^{6}-1360 \, k^{4}-1063 \, k^{2}+3\right) \left(k-1\right)^{2} \left(k+1\right)^{2} K^{2} E^{2}}{23625 \, k^{8}}
        +\frac{64 (504 k^{8} - 1739 k^{6} - 975 k^{4} - 865 k^{2} + 3) (k - 1)^{3} (k + 1)^{3} K^{3} E}{70875 k^{8}}
         \frac{16 (1011 k^6 + 599 k^4 + 697 k^2 - 3) (k - 1)^4 (k + 1)^4 K^4}{70875 k^8}
> Ct(5,5);
```

```
256(262 - 1411795 k^4 - 1417235 k^6 - 1102985 k^{14} + 9340 k^2 - 7179887 k^{10} + 26133515 k^{12}
        -20785 k^{18} - 2293735 k^8 - 133795 k^{16} + 12 k^{20}) E^5 / (781396875 k^{12}) - 256
        (96 k^{16} + 811 k^{14} + 8548 k^{12} - 363315 k^{10} - 165262 k^8 - 92539 k^6 - 44064 k^4 + 355 k^2 + 10)
        (k-1)^2(k+1)^2KE^4/(6251175k^{12})-256(360k^{18}+651k^{16}+31658k^{14}-6410543k^{12})
        +6389472 k^{10} + 2643313 k^8 + 1923170 k^6 + 1729647 k^4 - 15796 k^2 - 476) (k-1)^2 (k+1)^2
        K^{2}E^{3} / (156279375 k^{12}) + 512 (270 k^{16} + 2523 k^{14} + 1010246 k^{12} - 1920319 k^{10} - 870116 k^{8}
        -707955 k^{6} - 667762 k^{4} + 7159 k^{2} + 226) (k-1)^{3} (k+1)^{3} K^{3} E^{2} / (156279375 k^{12}) - 512
       (135 k^{14} - 122352 k^{12} + 551498 k^{10} + 258369 k^8 + 239203 k^6 + 256106 k^4 - 3204 k^2 - 107)
       (k-1)^4 (k+1)^4 K^4 E / (156279375 k^{12}) + 256
       (225 k^{12} - 616911 k^{10} - 284740 k^8 - 286190 k^6 - 391095 k^4 + 5645 k^2 + 202) (k-1)^5 (k+1)^5
       K^5 / (781396875 k^{12})
                                                     \frac{E}{k} + \frac{(k-1)(k+1)K}{k}
  > C(2,2);
                          -\frac{\left(-5+k^{2}\right)E^{2}}{3k^{2}}+\frac{8(k-1)(k+1)KE}{3k^{2}}+\frac{(k-1)^{2}(k+1)^{2}K^{2}}{k^{2}}
> C(3,3);
   \frac{4 \left(-96 \, k^2+10 \, k^6+1+21 \, k^4\right) E^3}{135 \, k^5} - \frac{4 \left(k-1\right) \left(k+1\right) \left(k^6+3 \, k^4-69 \, k^2+1\right) K E^2}{45 \, k^5}
      +\frac{4 \left(k^{4}+48 k^{2}-1\right) \left(k-1\right)^{2} \left(k+1\right)^{2} K^{2} E}{45 k^{5}}+\frac{4 \left(33 k^{2}-1\right) \left(k-1\right)^{3} \left(k+1\right)^{3} K^{3}}{135 k^{5}}
> C(4,4):
\frac{16 \left(-549 \, k^2-1977 \, k^8+21773 \, k^4-1549 \, k^{10}-47-5366 \, k^6+3 \, k^{12}\right) E^4}{70875 \, k^8}
         \frac{128 (k-1) (k+1) (129 k^{10} + 134 k^8 + 658 k^6 - 7332 k^4 + 245 k^2 + 22) K E^3}{128 (k-1) (k+1) (129 k^{10} + 134 k^8 + 658 k^6 - 7332 k^4 + 245 k^2 + 22) K E^3}
        \frac{32 (30 k^{10} - 81 k^8 + 70 k^6 - 9704 k^4 + 428 k^2 + 41) (k - 1)^2 (k + 1)^2 K^2 E^2}{2}
      +\frac{64 (45 k^{8}+111 k^{6}+6389 k^{4}-363 k^{2}-38) (k-1)^{3} (k+1)^{3} K^{3} E}{70875 k^{8}}
        -\frac{16 \left(9 k^6-843 k^4+59 k^2+7\right) \left(k-1\right)^4 \left(k+1\right)^4 K^4}{14175 k^8}
> C(5,5);
```

```
256(12-133795 k^4-1102985 k^6-1417235 k^{14}-20785 k^2-7179887 k^{10}-2293735 k^{12}
      +9340 k^{18} + 26133515 k^8 - 1411795 k^{16} + 262 k^{20}) E^5 / (781396875 k^{13}) + 256 (k-1)
      (k+1)(12k^{20}+715k^{18}-301320k^{16}-205360k^{14}-475660k^{12}-2228562k^{10})
      +16836940 k^{8} - 909560 k^{6} - 115920 k^{4} - 18385 k^{2} + 12) K E^{4} / (156279375 k^{13}) - 256 (
      24 k^{18} + 111337 k^{16} - 89860 k^{14} - 41517 k^{12} + 943946 k^{10} - 21491273 k^8 + 1463928 k^6
      +196741 k^4 + 32330 k^2 - 24) (k-1)^2 (k+1)^2 K^2 E^3 / (156279375 k^{13}) - 256 (14157 k^{16})
      -83180 k^{14} - 131273 k^{12} - 20398 k^{10} - 13698717 k^8 + 1145440 k^6 + 162833 k^4 + 28250 k^2
      -24)(k-1)^{3}(k+1)^{3}K^{3}E^{2}/(156279375k^{13})+256
      (14169 k^{14} + 12352 k^{12} + 35277 k^{10} + 4382564 k^8 - 434621 k^6 - 65328 k^4 - 12265 k^2 + 12)
      (k-1)^4 (k+1)^4 K^4 E / (156279375 k^{13}) - 256
      (17715 k^{12} + 65501 k^{10} - 2824190 k^8 + 320730 k^6 + 50375 k^4 + 10585 k^2 - 12) (k-1)^5
      (k+1)^5 K^5 / (781396875 k^{13})
Non diagonal correlation functions
  > map(factor,collect(Ct(0,1),[E,K],distributed));
                                      -\frac{(k-1)\sqrt{k+1}K}{2} + \frac{\sqrt{k+1}}{2}
                 -\frac{E^2}{k} - \frac{2(k-1)(k+1)KE}{k} - \frac{(k+2)(k+1)(k-1)^2K^2}{2k} + \frac{k}{2} + \frac{1}{2}
 > map(factor,collect(Ct(0,2),[E,K],distributed));
                 -\frac{E^2}{k} - \frac{2(k-1)(k+1)KE}{k} - \frac{(k+2)(k+1)(k-1)^2K^2}{2k} + \frac{k}{2} + \frac{1}{2}
 > map(factor,collect(Ct(1,2),[E,K],distributed))
 \frac{\sqrt{k+1} E^2}{k} + \frac{(k-1)(k+3)\sqrt{k+1} E K}{2 k} + \frac{(k-1)\sqrt{k+1} E}{2 k} + \frac{(k-1)^2(k+1)^{(3/2)} K^2}{2 k}
      -\frac{(k-1)(k+1)^{(3/2)}K}{2k}
 > map(factor,collect(Ct(0,3),[E,K],distributed));
 \frac{2(k-1)\sqrt{k+1}E^3}{k^2} + \frac{(k-1)\sqrt{k+1}(k^2-6k-11)E^2K}{2k^2} - \frac{\sqrt{k+1}(k^2+6k+1)E^2}{2k^2}
      -\frac{(3 k+5) (k-1)^2 (k+1)^{(3/2)} K^2 E}{L^2} - \frac{(3 k+1) (k-1) (k+1)^{(3/2)} E K}{L^2}
      -\frac{(k+3)(k-1)^3(k+1)^{(5/2)}K^3}{2k^2} - \frac{(k-1)^2(k+1)^{(7/2)}K^2}{2k^2} + \frac{(k-1)(k+1)^{(5/2)}K}{2k}
 > map(factor,collect(Ct(1,3),[E,K],distributed));
```

```
-\frac{(k^2-6 \, k-11) \, E^3}{3 \, k^2} + \frac{2 \, (k-1) \, (3 \, k+13) \, (k+1) \, K \, E^2}{3 \, k^2}
       +\frac{2(k+1)(k^2+9k+10)(k-1)^2K^2E}{2k^2}+\frac{(k+1)(2k^2-3k-1)E}{2k^2}
       +\frac{(3 k+5) (k+1)^2 (k-1)^3 K^3}{3 k^2} -\frac{(3 k+1) (k-1) (k+1)^2 K}{3 k^2}
  > map(factor,collect(Ct(2,3),[E,K],distributed))
  \frac{(k-1)(k^2+6k+1)\sqrt{k+1}E^3}{3k^3} + \frac{(k-1)(k^4+15k^3-k^2-39k-8)\sqrt{k+1}E^2K}{9k^3}
       -\frac{(k^2+1)(k^2-6k+1)\sqrt{k+1}E^2}{9k^3}+\frac{(k+1)^{(3/2)}(3k^3-k^2-27k-7)(k-1)^2K^2E}{9k^3}
       +\frac{(k-1)(k+1)^{(3/2)}(3k^3-2k^2+9k-2)EK}{9k^3}-\frac{2(3k+1)(k+1)^{(5/2)}(k-1)^3K^3}{9k^3}
       +\frac{(3 k-1) (k-1)^2 (k+1)^{(5/2)} K^2}{9 k^3}
>
  > map(factor,collect(C(0,1),[E,K],distributed));
                                             \frac{\sqrt{k+1}\,\left(k-1\right)K}{2\,\sqrt{k}} + \frac{\sqrt{k+1}}{2\,\sqrt{k}}
   > map(factor,collect(C(0,1),[E,K],distributed));
                                               \frac{\sqrt{k+1}(k-1)K}{2\sqrt{k}} + \frac{\sqrt{k+1}}{2\sqrt{k}}
   > map(factor,collect(C(0,2),[E,K],distributed));
                                          -\frac{E^2}{k} + \frac{(k+1)(k-1)^2 K^2}{2 k} + \frac{k+1}{2 k}
   > map(factor,collect(C(1,2),[E,K],distribut
   \frac{\sqrt{k+1} E^2}{t^{(3/2)}} + \frac{(k-1)(k+3)\sqrt{k+1} E K}{2t^{(3/2)}} - \frac{(k-1)\sqrt{k+1} E}{2t^{(3/2)}} + \frac{(k-1)^2(k+1)^{(3/2)} K^2}{2t^{(3/2)}}
         +\frac{(k-1)(k+1)^{(3/2)}K}{2 \iota^{(3/2)}}
   > map(factor,collect(C(0,3),[E,K],distributed));
   -\frac{2(k-1)\sqrt{k+1}E^{3}}{t^{(5/2)}} - \frac{(k-1)\sqrt{k+1}(k^{2}-6k-11)E^{2}K}{2t^{(5/2)}} - \frac{\sqrt{k+1}(k^{2}+6k+1)E^{2}}{2t^{(5/2)}}
        +\frac{(3 k+5) (k-1)^2 (k+1)^{(3/2)} K^2 E}{t^{(5/2)}} -\frac{(3 k+1) (k-1) (k+1)^{(3/2)} E K}{t^{(5/2)}}
        +\frac{(k+3)(k-1)^3(k+1)^{(5/2)}K^3}{2^{k^{(5/2)}}}-\frac{(k-1)^2(k+1)^{(7/2)}K^2}{2^{k^{(5/2)}}}-\frac{(k-1)(k+1)^{(5/2)}K}{2^{k^{(3/2)}}}
```

$$\begin{array}{l} + \frac{(k+1)^{(5/2)}}{2\,k^{(3/2)}} \\ > & \max \left(\operatorname{factor}, \operatorname{collect}\left(\operatorname{C}\left(1,3 \right), \left[\operatorname{E}, \operatorname{K} \right], \operatorname{distributed} \right) \right); \\ \frac{(-1+6\,k+11\,k^2)\,E^3}{3\,k^3} + \frac{(k-1)\,(k+1)\,(7\,k^2+12\,k-3)\,K\,E^2}{3\,k^3} \\ + \frac{(k+3)\,(k+1)\,(k^2+2\,k-1)\,(k-1)^2\,K^2\,E}{3\,k^3} - \frac{(k+1)\,(k^2+3\,k-2)\,E}{3\,k^2} \\ + \frac{(k+1)^2\,(k-1)^4\,K^3}{3\,k^3} + \frac{2\,(k-1)\,(k+1)^2\,K}{3\,k^2} \\ \\ > & \max \left(\operatorname{factor}, \operatorname{collect}\left(\operatorname{C}\left(2,3 \right), \left[\operatorname{E}, \operatorname{K} \right], \operatorname{distributed} \right) \right); \\ - \frac{(k-1)\,(k^2+6\,k+1)\,\sqrt{k+1}\,E^3}{3\,k^{(7/2)}} - \frac{(k-1)\,(k^4+15\,k^3-k^2-39\,k-8)\,\sqrt{k+1}\,E^2\,K}{9\,k^{(7/2)}} \\ - \frac{(k^2+1)\,(k^2-6\,k+1)\,\sqrt{k+1}\,E^2}{9\,k^{(7/2)}} - \frac{(k+1)^{(3/2)}\,(3\,k^3-k^2-27\,k-7)\,(k-1)^2\,K^2\,E}{9\,k^{(7/2)}} \\ + \frac{(k-1)\,(k+1)^{(3/2)}\,(3\,k^3-2\,k^2+9\,k-2)\,E\,K}{9\,k^{(7/2)}} + \frac{2\,(3\,k+1)\,(k+1)^{(5/2)}\,(k-1)^3\,K^3}{9\,k^{(7/2)}} \\ + \frac{(3\,k-1)\,(k-1)^2\,(k+1)^{(5/2)}\,K^2}{9\,k^{(7/2)}} \end{array}$$

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